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CURRENT STATUS IN FINE CERAMICS

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SCIENCE & TECHNOLOGY JAPAN

CURRENT STATUS IN FINE CERAMICS

926C0044 Tokyo MUKI SHINSOZAI SANGYO TAISAKU CHOSA ITAKU CHOSA KENKYU
HOKOKUSHO in Japanese Mar 91 pp 1-225

[Report on Inorganic New Materials (Fine Ceramics) Industrial Policy Investigation prepared by the Japan Fine Ceramics Association under MITI contract]

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Current Status, Future of Fine Ceramics

926C0044 Tokyo MUKI SHINSOZAI SANGYO TAISAKU CHOSA ITAKU CHOSA KENKYU
HOKOKUSHO in Japanese Mar 91 pp 1-225

[Article: "Current Status and Future of Fine Ceramics Materials Science"]

[Excerpts] 5.1 Structural Ceramics

5.1.1 Material Process

(1) Monolithic Materials

The ultimate dream and goal of the developmental activity for people engaged in the research and manufacture of ceramics is to freely control the organization and composition of ceramics and its structure, as needed. Development of technology for controlling the properties of ceramics has been going on centered on those ceramics for use as electronic materials, magnetic materials or optical materials, but great progress has also been achieved in structural ceramics in recent years. The targets of controls have reached the submicron level for practical uses, and the direction of development is nearing the nanometer range.

Due to advances in synthesis technology and analysis technology achieved over the past 20 years, great improvements have been made in the material characteristics of the raw material powders (with respect to particle size, purity, etc.). For example, alumina is widely used not only as the structural material for a variety of applications, such as for abrasion resistance, but also as the raw material for IC substrates and electronic and optical materials such as Na lamps. Great advances have been made with respect to the higher material purity and smaller material grain size, thereby yielding controls of the powder characteristics at fairly higher levels of accuracy.

Figure 5.1.1 shows shapes of grain-size controlled, high-purity alumina powders. The grain diameters were obtained from BET relative surface areas. It is well known that the finer the grains, the easier it is to sinter, and lower sintering temperatures not only improve the quality of the sintered body with respect to such properties as mechanical strength and surface accuracy but also facilitate the ease of controlling its microcrystalline structure and its blending.

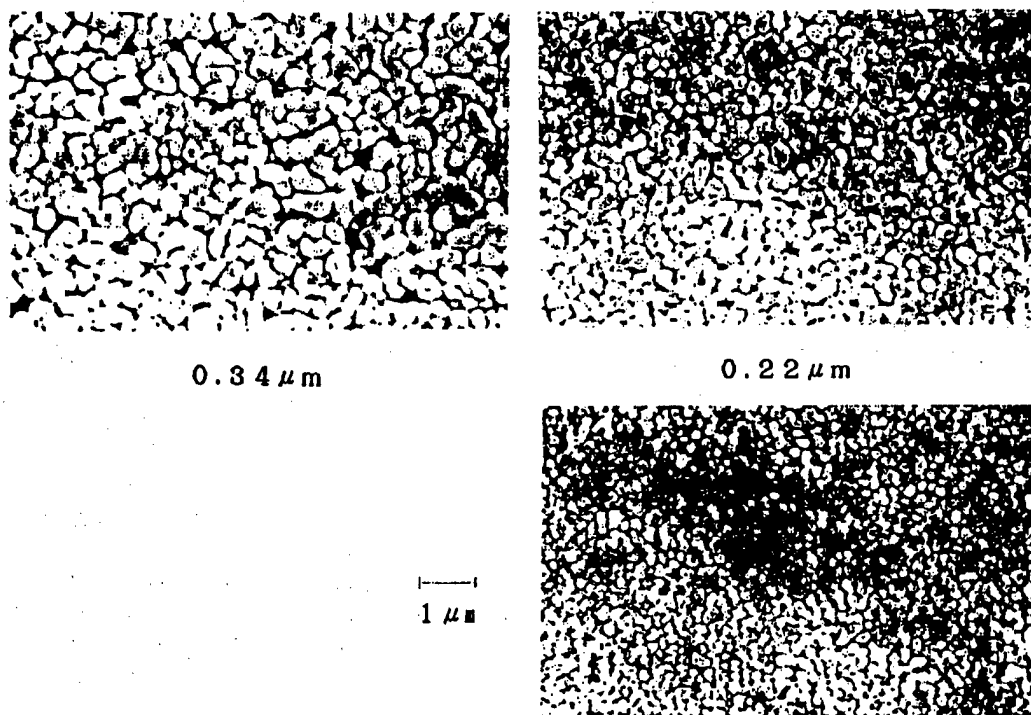


Figure 5.1.1.1 Shapes of Grain-Size-Controlled, High-Purity Alumina Powders

Figure 5.1.1.2 shows sintering characteristics of alumina powder. Here, the temperature at which sintering starts is the temperature corresponding to 0.5 percent shrinkage rate while the temperature at which sintering terminates is the temperature corresponding to 95 percent relative density. As is duly expected from their smaller grain sizes, alumina of about $0.3 \mu\text{m}$ starts sintering at below $1,000^\circ\text{C}$.

Figure 5.1.3 shows the dependence of relative density on temperature in sintered bodies prepared by different processing methods. The differences in relative density come not merely from the differences in the density of forming but also are affected by the differences in how closely the microscopic network of grains is packed together.

Consequently, development of the techniques to estimate how close the microscopic network of grains is packed together, based on the fine particle characteristics, will become important.

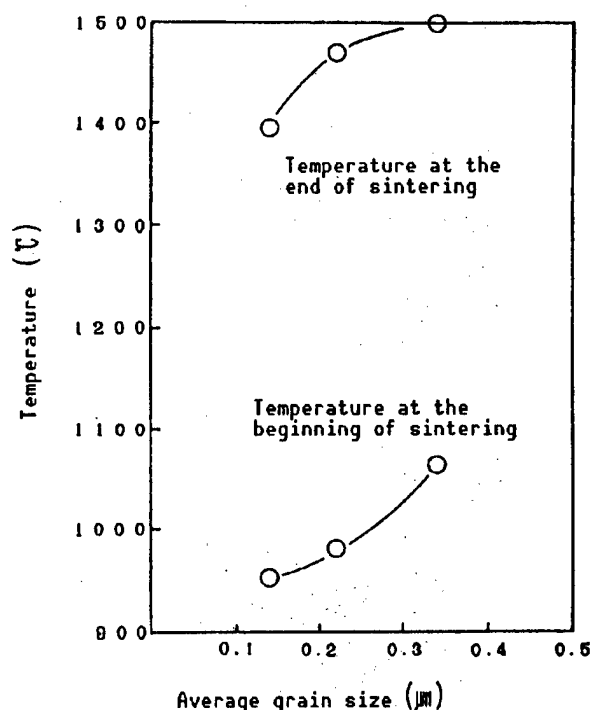


Figure 5.1.1.2 Dependence of Sintering Temperature on Grain Diameter in High-Purity, Fine-Grain Alumina

Figure 5.1.1.4 shows the relationship between bending strengths and defect sizes in sintered bodies of alumina. As expected, higher strengths are obtained with decreasing flaw sizes. However, strength-governing defects are rarely to be found in sintered bodies with a density in excess of 100 kg/mm², and they are considered to have come from the sintered body's defects at the grain diameter level or its surface defects. This corresponds to the aforementioned differences in the

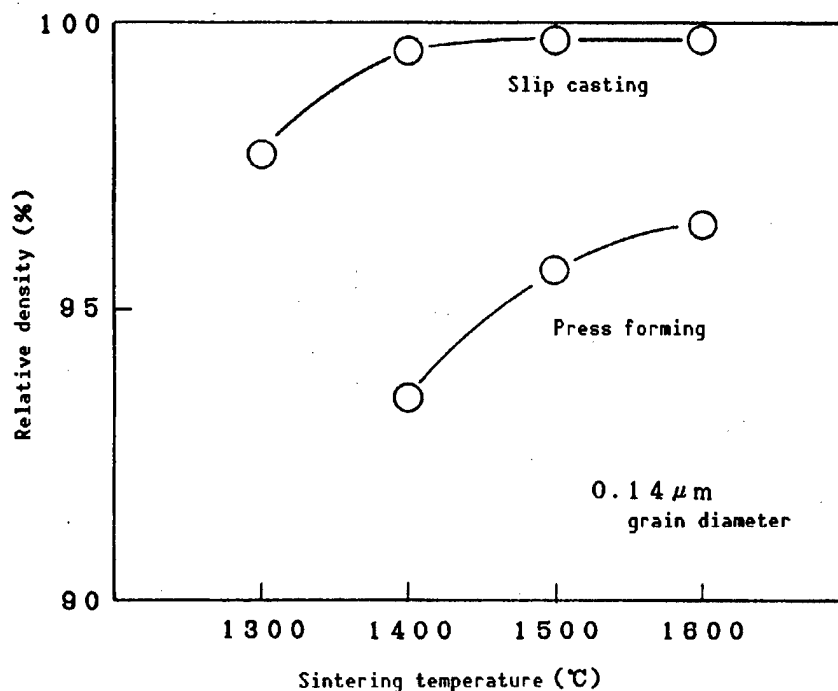


Figure 5.1.1.3 Relative Density of High-Purity, Fine-Grain Alumina Is Affected by Processing Methods

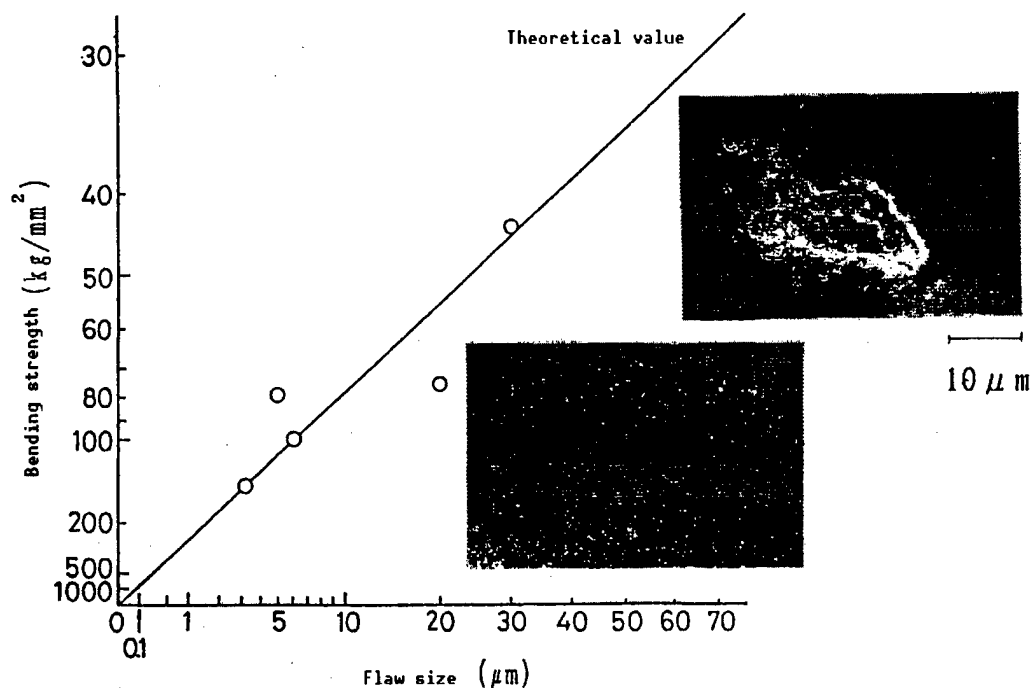


Figure 5.1.1.4 Dependence of Bending Strengths on Flaw Sizes in High-Purity, Fine-Grain Alumina

microscopic network of grains, brought about by different processing methods, thereby suggesting the possibility that the origin of defects may be traced back to differences in particle characteristics.

Regarding the packing properties of a class of particles ranging in size from submicron to nanometer, interesting studies have been made by Aksay, et al. By taking advantage of lattice-gas models, they have developed correlation diagrams of colloidal systems of spherical particles of a uniform particle size. From the results of observations of close-packed structures of particles, they have confirmed that in colloidal systems of fine particles from submicron down to nanometer, there occur hierarchical coagulations, and they are studying the correspondence between the hierarchical coagulations and the correlation diagrams. Figure 5.1.1.5 shows a nonequilibrium correlation diagram for a colloidal system. Here, V is the potential of interaction between particles, k is the Boltzmann constant, and T is the temperature. It suggests that a high-density dispersion is not realized in either of the spheres where electrostatic interaction is at play, the high V/kT and the low V/kT , but that a high-density colloidal dispersion may be found in the intermediate sphere.

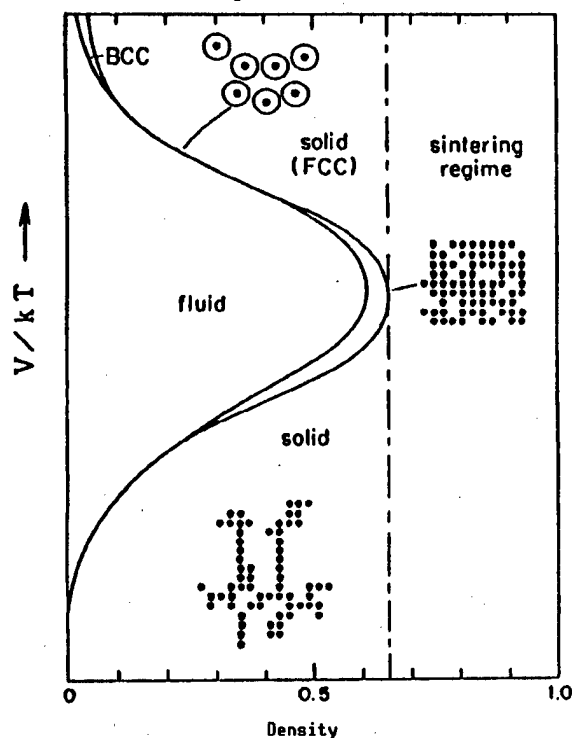


Figure 5.1.1.5 Nonequilibrium Correlation Diagram of Colloidal System

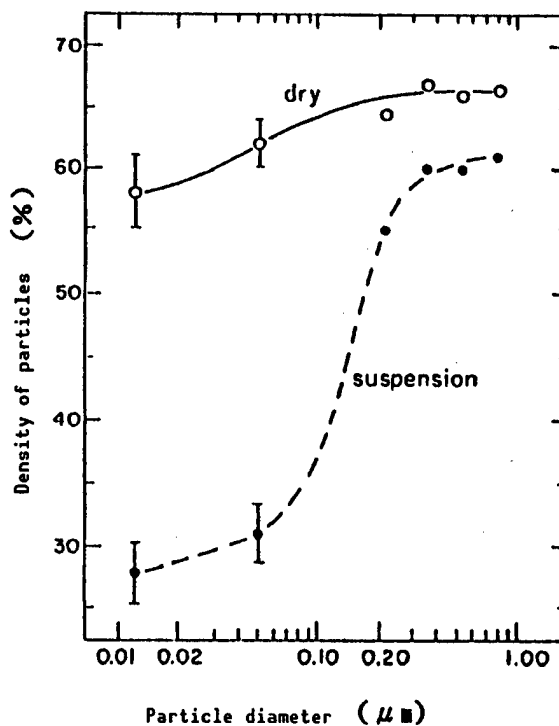


Figure 5.1.1.6 Dependence of Particle Density on Particle Diameter in α -Alumina and Aluminum Hydroxide

Figure 5.1.1.6 gives the maximum particle densities (viscosity: below 1 Pa/sec) available for α -alumina (α - Al_2O_3) and the aluminum hydroxide ($\text{Al}(\text{OH})_3$). It shows that sharp drops in particle density occur when particles are below 0.1 μm in diameter and that the density gains when it is dry.

As described above, studies on the technology of estimating the dispersion of particles—further the packing structure of particles—are progressing and the next logical goal should be the development of the technique of utilizing the estimate in obtaining a uniform and high-density dispersion or packing (forming) of particles ranging from submicron to nanometer in size.

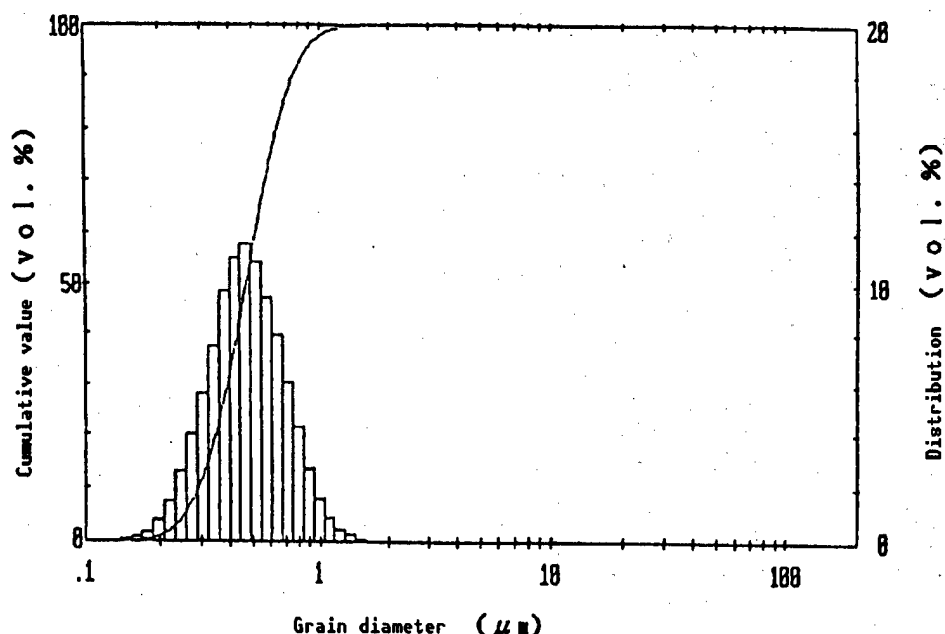


Figure 5.1.1.7 Particle Size Distribution in High-Purity, Fine-Grain Alumina

Particle diameters of these powders are controlled by the synthesis conditions and/or the pyrolysis and heat treatment conditions, and show sharp distributions. However, if further progress is to be achieved in the technique of controlling the organization and structure, it is considered that a great task that remains to be solved is how to synthesize particles with a still sharper particle size distribution while controlling their shapes.

(2) Ceramic-Based Composite Materials

(a) Process and physical properties

The following are examples in which, as described in paragraph 3.6, different intermediate techniques can be employed in manufacturing to obtain sintered bodies with greatly differing physical properties.

For example, hot isostatic pressing (HIP), a technique that is widely used, makes it possible to eliminate from the sintered body the kind of flaws that cannot be removed with the conventional sintering method, by subjecting it to treatment under high pressure, thereby helping raise its material properties and reliability. In particular, the industrial use of HIP in oxide ceramics is used in a broad range of applications beginning with the technique's use in the making of alumina tools in 1976 and its application to ferrite and lead zirconate titanate (PZT). However, it is reported that in some materials, the use of Ar gas as a pressure medium gives rise to reductions or decomposition reactions, thereby lowering rather than strengthening their properties or causing a deterioration in their surface quality.

In order to solve these problems the equipment (O_2 -HIP) has been developed that enables the use of a mixed gas of argon and oxygen as the pressure medium. Using the equipment, studies have been made on what effects changes in the amounts of oxygen and other elements have on the properties (principally, density, three-point bending strength, etc.) of an oxide ceramic—alumina- and yttrium-based partially stabilized zirconium.

The findings have been made public. On the other hand, Figure 5.1.1.8 shows the relationship between hardness and density in a high-purity sintered body of alumina when it is subjected to HIP treatment: both the Ar-HIP and O_2 -HIP treatment yield about the same densities, but in the latter the effect on the matrix is less severe and improvements of more than 10 percent in Vickers hardness are obtained after the HIP treatment, compared with before treatment. These suggest that similar results may be obtained in other oxides and composite materials with oxide matrixes as their base.

High-pressure synthesis technology of diamond has helped propel advances in materials development in high-pressure generation technology. In retrospect, the successful synthesis of diamond in 1954 was nothing but a thermal dissolution and precipitation reaction of carbon under stabilized temperature-pressure conditions. However, the process has made it possible to obtain diamond particles from graphite in short hours using ferrous metals as the catalyst. Figure 5.1.1.9 shows a diagram of carbon and the nickel-carbon eutectic line. In the hatched area, the diamond is stable in terms of thermotics and its synthesis is possible at temperatures higher than the Ni-C eutectic temperature.

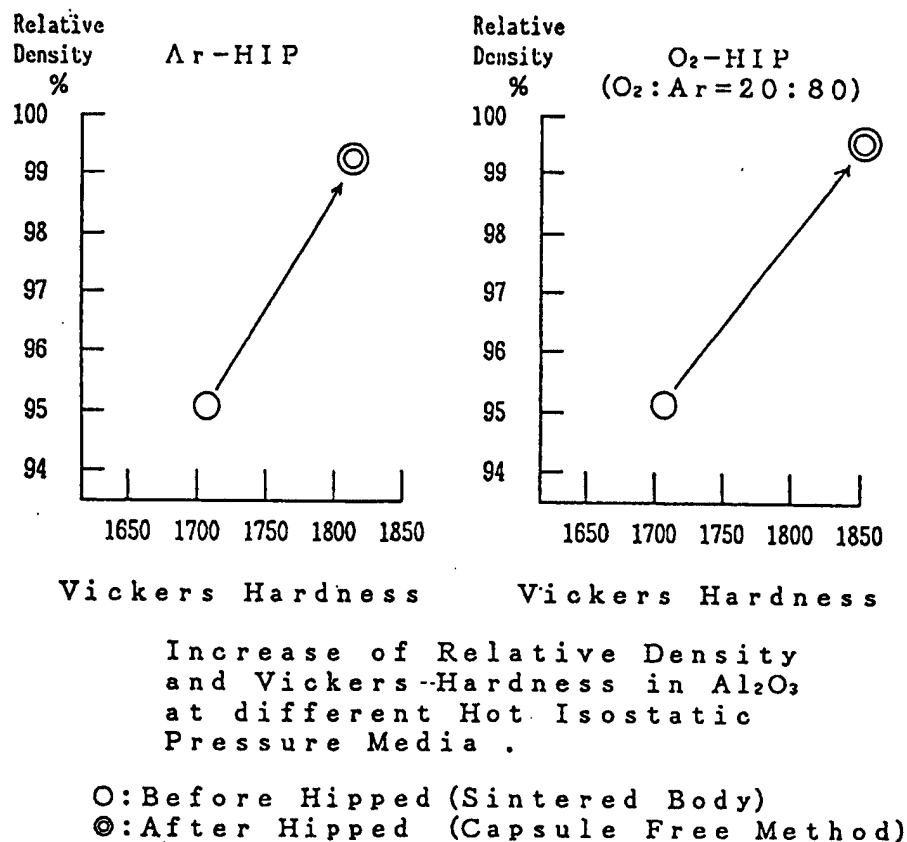


Figure 5.1.1.8 Different Media Have Different Effects on HIP Processed Alumina

Full attention is now being paid to the methods of controlling the pressure and temperature throughout the course of the synthesis in question. As a result, in diamond synthesis as shown in Figure 5.1.1.10, it has become apparent that there are differences in the crystal morphology and the number and size of crystal grains between the following two processes— 1) the temperature is raised to a desired temperature under the pressure condition in which diamond is thermodynamically stable; and 2) the temperature is raised or lowered to a desired temperature under pressures that are below the pressure in which graphite is thermodynamically stable and the pressure is restored to the level where diamond is generated. Furthermore, it has become apparent that how the speed of raising or lowering the temperature is controlled yields a great effect on the properties of the crystals. Grinding grains of limited sizes are finding many applications, and high-quality diamonds of a uniform grain size are now obtained by using the control procedure (C) along the "graphite-diamond equilibrium line" but the technology still has room for improvement. In the latter half of the 1960s, with the objective of improving the flaws of diamond such as brittleness while maintaining the superb characteristics of its single crystals, attempts were made to synthesize sintered bodies of diamonds, and GE succeeded in commercializing a product that was synthesized by sintering WC-Co and diamond simultaneously under high-temperature and high-pressure conditions in which diamond is thermodynamically stable.

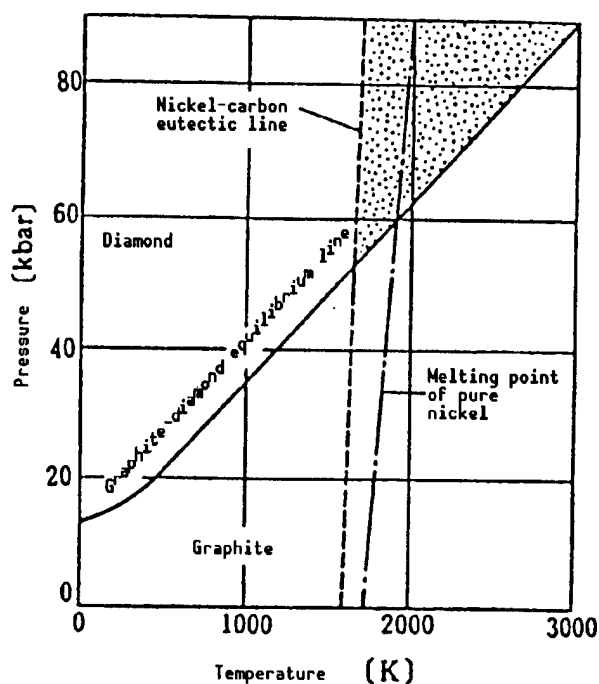


Figure 5.1.1.9 Diagram of Carbon and Nickel-Carbon Eutectic Line

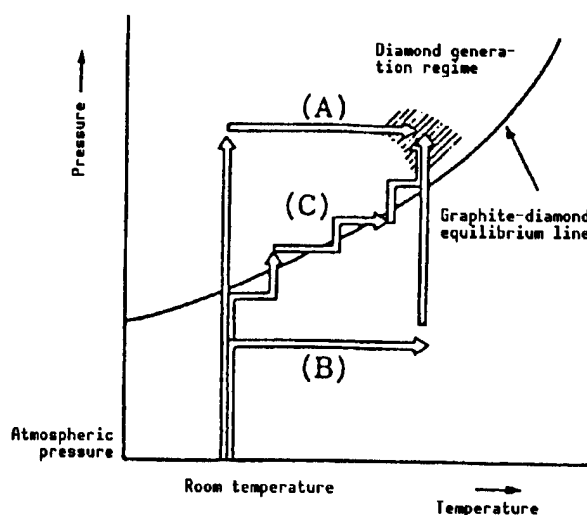


Figure 5.1.1.10 Control Procedures of Pressure and Temperature in Diamond Synthesis

(b) Composite materials and their physical properties

As with metal matrix composites (MMC), in order to impart composite ceramics with the required properties, the first requirement is the development of excellent materials, followed by the development of technology to blend and

fabricate those materials into a product. Furthermore, the theories that enable the properties of such composite ceramics to be analyzed will have to be established. Until now the goals have been attained empirically through trial and error experiments, but the processes are highly inefficient in most cases.

The basic ideas about composite materials with a ceramic matrix are described in paragraph 3.6, and here the relationship between the four-point bending strength and K_{IC} in the representative composite TiC/Al₂O₃ is given in Figure 5.1.1.11. The two properties gain the highest values when the ratio of dispersed particles (TiC) is in the neighborhood of 30 wt%.

This suggests that similar results may be obtained when particles of other carbides in place of TiC are dispersed. Similarly, many studies have been made on the details of the mechanisms of destruction in fiber-reinforced SiCw/Al₂O₃ and SiCw/Si₃N₄.

Here, as shown in Figure 5.1.1.12, as for the relationship between the average diameter d of SiC whiskers and K_{IC} , the K_{IC} of Al₂O₃ itself was 3.0 MPa·m^{1/2}, but little improvement is observed in the fracture toughness when the whisker diameter is in the 0.3~0.5 μm range. Again, when the whisker diameter is 1.88 μm, the effect is great, with K_{IC} rising to 4.95 MPa·m^{1/2}, and in this range, K_{IC} goes up in proportion to the whisker diameter of SiC d to the 1/2 power.

Tohoku University at present is developing a materials development support system for various advanced materials beginning with ceramic matrix composites (CMC). Targeted for accomplishment over the coming three years, the system will enable such mechanical and thermal characteristics as the stress-strain curve, fracture strength resistance curve, fracture toughness, thermal expansion coefficient, heat conductivity, energy absorption characteristics,

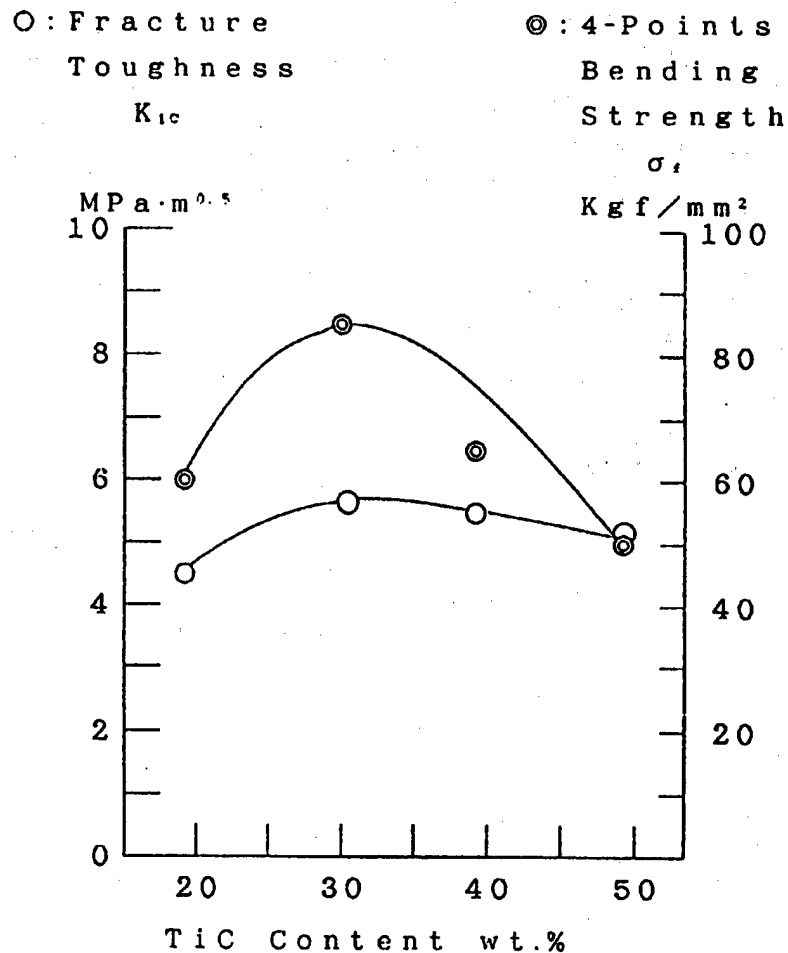


Figure 5.1.1.11 Relationship Between TiC Content and Four-Point Bending Strength and K_{IC} in TiC/Al₂O₃

creep characteristics, and stress corrosion characteristics to be displayed on a workstation class computer. It will enable materials experiments to be conducted on the screen of a computer system, that is, data input into the computer system, such as properties and shapes of component elements of a material and the natures of interfaces, are immediately displayed on the screen as the material's properties. What is specific about this system is that when the microscopic properties, shapes, and interfaces on the orders of grains and grain boundaries rather than the Å levels for electrons and particles of the constituent elements of a composite to be generated are input, it enables the composite's properties to be known immediately. The system not only will make it possible to shorten the time needed for development of advanced materials but will also make it possible for people who have neither highly advanced professional knowledge nor experience to engage in development. The technical parameters incorporated in the system will greatly help its use as a practical support system.

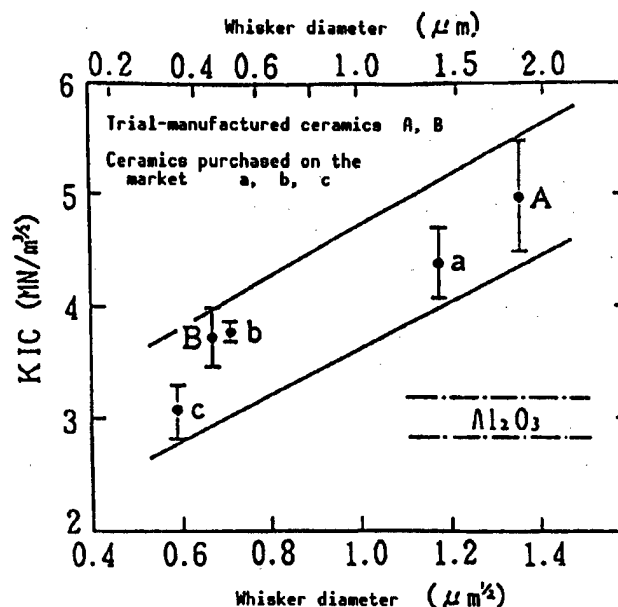


Figure 5.1.1.12 Relationship Between Fracture Toughness K_{IC} and Whisker Diameter d in Al_2O_3 20 vol% SiC Whisker Ceramics

5.1.2 Parts Design and Manufacture

This section describes applications of structural ceramics for use as automotive engine parts, and relates the current state of how an approach based on materials science is being employed for solving the related problems, i.e., how to design parts and ensure their reliability, as well as how to manufacture those parts, and their future prospects.

(1) Current State of Structural Ceramics

Structural ceramics including silicon nitride and silicon carbide show excellent heat-, corrosion- and abrasion-resistance properties not found in metallic materials, so attempts have actively been made to develop ceramic parts for automobile engines. Table 5.1.2 shows major ceramic engine parts that are finding practical use at present. What is noteworthy about the table is that except for the port liner of aluminum titanate developed by Porsche, all have been developed by Japanese car makers using silicon nitride. the advantages and problems of ceramic engine parts are considered in the following.

Table 5.1.2.1 Major Ceramic Parts That Have Found Practical Applications

Parts	Material	Car maker	Ceramics maker	Year of mounting
Glow plug	Silicon nitride	Isuzu Motors Mitsubishi Motor Nissan Motor	Kyocera Kyocera NGK Spark Plug	1981 1983 1985
Hot plug	Silicon nitride	Isuzu Motors Toyota Motor Mazda Motor	Kyocera Toyota Motor NGK Insulators	1983 1984 1986
Rocker arm	Silicon nitride	Mitsubishi Motor	NGK Insulators	1984
Port liner	Aluminum titanate	Porsche	"Fueldmule Hext"	1985
Turbo-charger rotor	Silicon nitride	Nissan Motor	NGK Spark Plug NGK Insulators	1985

A glow plug is a heater for preheating the combustion chamber when starting a diesel engine. Conventional metallic plugs need 20-30 seconds of preheating in aiding the engine in starting, but the higher heat resistance of ceramic plugs enables the preheating time to be shortened.

A hot plug is a part that makes up the eddy current chamber in a diesel engine. The high-heat resistance and high insulation properties of silicon nitride help reduce heat loss, which in turn has the advantage of improved fuel efficiency, reduced noise emitted by the engine in idling, and an enhanced ease of starting the engine. Also, higher operating temperatures help increase output power and reduce emission of particulates.

Conventional rocker arm chips made of metals easily wear off in engines on taxis that are frequently kept in a state of idling, but ceramic chips enable the wear and tear to be reduced, thereby reducing the need to replace them so often. An added advantage is that the lighter chips help improve the valve mechanisms when the engine is operating at high speeds.

Conventional turbochargers made of metallic components had problems of turbo lags, but the development of turbochargers using silicon nitride—and the resultant reduction in their weight—have made it possible to reduce the turbo lag, thereby contributing to an increase in the engine's acceleration.

In addition to the parts made of structural ceramics described above, structural ceramics have bright prospects in their uses in gas turbine engine parts. For gas turbine engines to be put to practical use, the fuel efficiency and output power of the engine need to be increased by raising its operating

temperature, and in this respect, the use of ceramics featuring excellent heat resistance as the structural material of the engine is highly effective.

As described above, structural ceramics are already finding use as the structural material for automotive engine parts. However, if their use is to further expand, structural ceramics will need additional improvements with respect to design technology, material characteristics, manufacturing process, and evaluation technology. The following describes the problems with structural ceramics and the directions of approaches toward their solution from the perspective of materials science.

(2) Current State of Materials Science in the Field of Parts Design

When ceramics are to be used as the structural material of engine parts, their applications will mostly be centered in environments featuring high temperatures and excessive abrasion. Under high-temperature environments, there are at work not only mechanical stresses but also thermal stresses, so the parts need to withstand complex combinations of such stresses. This section describes the ideas on the design of engine parts for use in high-temperature environments and the current state of utilization of materials science in their design.

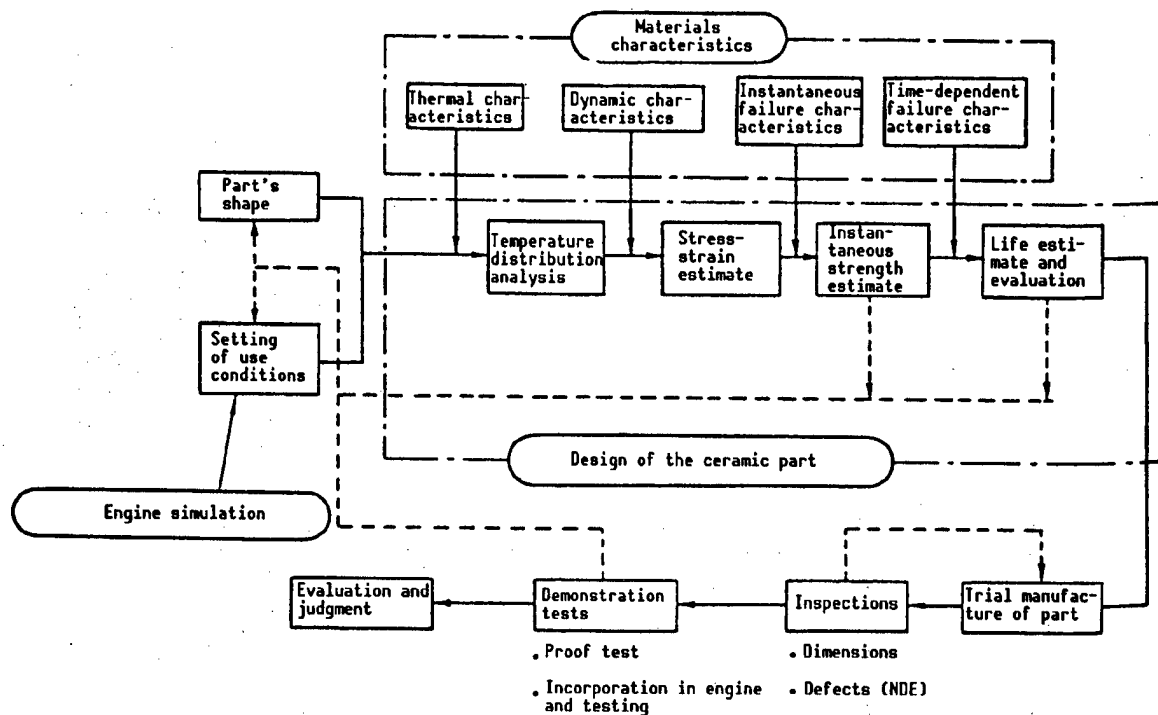


Figure 5.1.2.1 Flow Chart for Development of Ceramic Parts

Figure 5.1.2.1 shows a flow chart for the development of ceramic parts. In the development of ceramic-based engine parts, the thrust of research is directed more toward improvements on the existing metal parts with respect to performance and capabilities than toward fabricating brand new ceramic parts.

Therefore, the shapes and dimensions of the required parts are known in advance in most cases. These ceramic-based parts are put to use under new conditions. The greatest problem that a ceramic parts designer faces at present is that the boundary condition is unknown. The boundary condition will have to be clarified in experiments, but as of the design stage, much of it is unknown. When developing an engine part, simulations of the engine's performance are conducted to simulate the conditions in which the part will most likely be used (temperature, pressure, external force, etc.). From such data as the shape and dimensions of the part, the dynamic and thermal boundary conditions, and the physical property values of the ceramic material (the values of the testpieces are used for convenience), the temperature distribution, thermal stress, and mechanical stress are calculated by means of the finite element methods (three- and two-dimensional methods).

Once the stress distribution and temperature distribution in the entire area of the part resulting from the action of the combined stresses of the thermal and mechanical stresses working on the part are known, the part's average breaking strength (momentary strength) and probability of failure can be calculated using the Weibull statistical method (two parameters). When the probability of failure is higher than the assumed value, either changes are made on the shape of the part to reduce the stresses working on it, or a redesign of the part is needed by using materials with larger strengths. Once the momentary strength has attained the predetermined target in the repetition of such operations, the work proceeds to estimating the next lifetime.

Data is still skimpy on the failure mechanisms of ceramic parts that have gone through long hours of operation. The idea underlying ceramic parts design is based on the slow crack growth concept; that is, a flaw on the surface or inside of a ceramic part generated while it was being manufactured leads to a microscopic crack. Once the crack is subjected to stress, it propagates because of the concentration of stress at the tip, and when the crack propagation reaches a certain critical level, the part breaks down catastrophically. Here, the lifetime of a part is estimated in advance, and in case the part's probability of failure within its estimated lifetime is large, remedial measures are taken, such as redesigning its shape, reducing the stress working on it, altering its materials, or easing its use conditions. When designing a part, studies will also have to be made—in addition to the aforementioned measures for coping with the slow crack growth—on the effects of the material of the part and its operating temperature on the creep rupture and the deterioration of strength caused by oxidation, but there is little data available at present.

Once the dimensions, materials, and the manufacturing method of the part are established, the next process is its trial manufacture. Various problems also arise in the trial manufacturing phase, and the sizes and distributions of internal defects of the part and its reliability are determined by the quality of work in that phase.

The finished ceramic parts are first checked for their dimensions and external appearances to determine if they are fit for use in later tests, and only those judged to be of high quality undergo various kinds of tests, such as

testing the parts as stand-alone products, in their various combinations, and by actually incorporating them in an engine. However, many of these parts break down during the course of testing. Each time a failure occurs, research is done to determine the cause and the findings are relayed as feedback to the design group to improve their technology. However, the design technology is still immature and much improvement is needed.

(a) An example of the design of a turbocharger

Next, using a ceramic turbocharger as an example, the theory of design and the work's relation with computerized materials science are described. Ceramics are much more brittle than metals, and a local flaw in the rotor caused by the local maximum stress working on it is considered to lead to a failure of the entire rotor. Therefore, it is necessary to reduce the concentrations of stresses inside the rotor as much as possible while taking care that the aerodynamic characteristics will not be lost or will be decreased to the minimum. In conducting the stress calculations for the ceramic rotor, a part of the nine-vane rotor, equally divided into nine sections, was broken down into elements and the three-dimensional finite element method (NASTRAN) was employed. Results of representative stress distribution calculations are given in Figure 5.1.2.2.

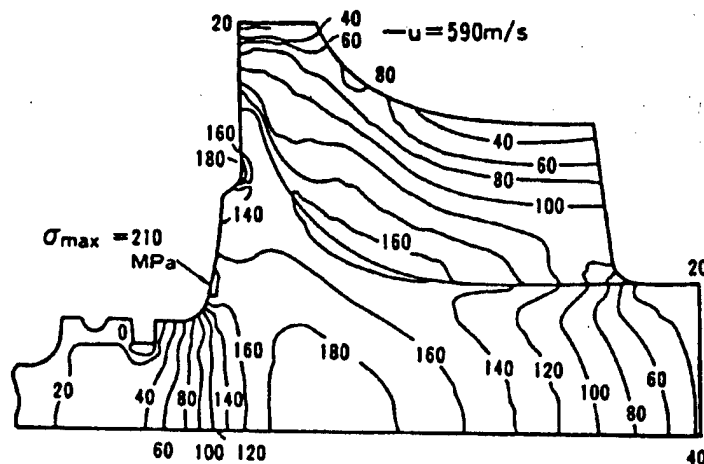


Figure 5.1.2.2 Centrifugal Stresses Working on Turbocharged Rotor

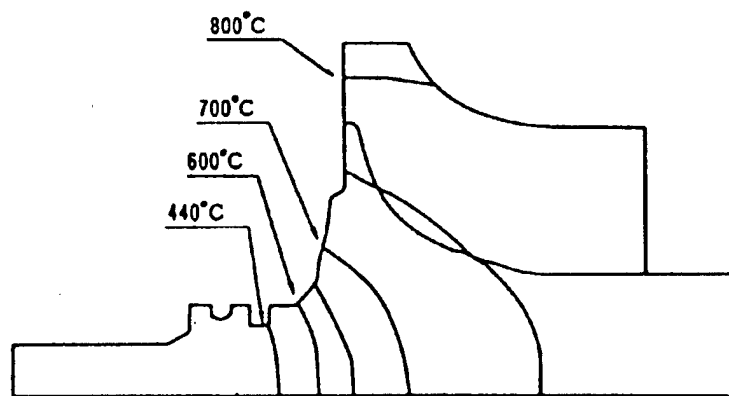
It shows the distribution of major maximum stresses and the maximum stresses are seen in the area from the back of the rotor to its axis.

Next, an example of calculations of a thermal stress distribution is given. Stresses generated when the turbine inlet temperature reached 900°C, a condition considered most demanding in terms of thermal stress under a normal state, were analyzed. Figure 5.1.2.3 gives a temperature distribution and the thermal stresses generated. The temperatures show a distribution roughly similar to the results of measurements of temperatures at the rotor's axis in the engine test. Under the temperature distribution, the values of the thermal stresses generated in the rotor, as opposed to the centrifugal stresses, are too large to be ignored. The actual stresses generated in the rotor are the syntheses of centrifugal stresses and thermal stresses, and the shape of a turbocharger is designed for taking advantage of the values of the synthesized stresses.

(b) Example of the design of a ceramic-metal bonding in a turbocharger

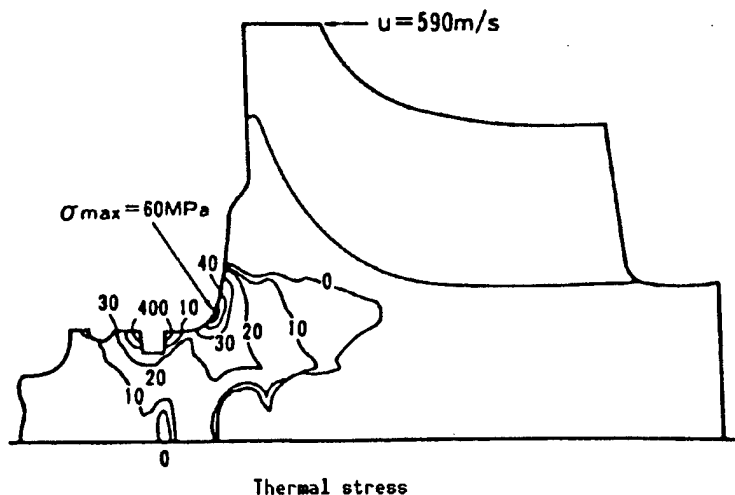
A rotor that is wholly made of ceramics, including its axis of rotation, gives rise to the probability of trouble: that is, should there occur a ceramic

failure, the outflowing of turbo lubricant into the exhaust system may give rise to trouble. Using an all-ceramic rotor may push up the cost of processing the axis, so a rotor is desired to be bonded with metals. Among the bonding mechanisms are the brazing method and the shrink-fit method. The brazing design is described.



Temperature distribution

In adopting the chemical bonding mechanism through brazing of ceramics with metals, there are two large technical tasks. One is to make sure that a chemical reaction occurs between silicon nitride—a highly covalent material that rarely reacts with other materials—and metals. This problem was solved by using a brazing material containing titanium as an activator in order to greatly improve its wettability to the surfaces of silicon nitride. The other problem is to inhibit the residual stresses at the bonded section which are caused by differences in physical properties between the silicon nitride and metal shaft, especially the large differences in the thermal expansion coefficients and in deformability, and which are generated in the cooling phase after the brazing and heating process.



Thermal stress

Figure 5.1.2.3 Temperature Distribution and Thermal Stress in Turbocharger

Figure 5.1.2.3 shows the distribution of calculations of residual stresses at joints. The figure shows that the adoption of a structure, in which a heat-resistant steel sleeve with a lower thermal expansion coefficient is arranged around the silicon nitride and metal shaft that are butt-joined via multiple buffer layers enables the harmful tensile stresses to be kept at lower values.

In order to reduce the residual stress, a structure is adopted in which multiple stress-mitigating layers are arranged between the silicon nitride and metal shaft. In designing the bonding scheme, model experiments using test-pieces and elasticity and plasticity analyses based on finite element analysis methods were conducted to determine the materials and shapes. Figure 5.1.2.4 shows the distribution of calculations of residual stresses at joints. The figure shows that the adoption of a structure, in which a heat-resistant steel sleeve with a lower thermal expansion coefficient is arranged around the silicon nitride and metal shaft that are butt-joined via multiple buffer layers enables the harmful tensile stresses to be kept at lower values.

(3) Current State of Materials Science in Design Reliability

A problem that engineers face when using ceramics as the structural material for engine components is that since ceramics are brittle materials, the usual effect—stress relaxation through plastic deformation—cannot

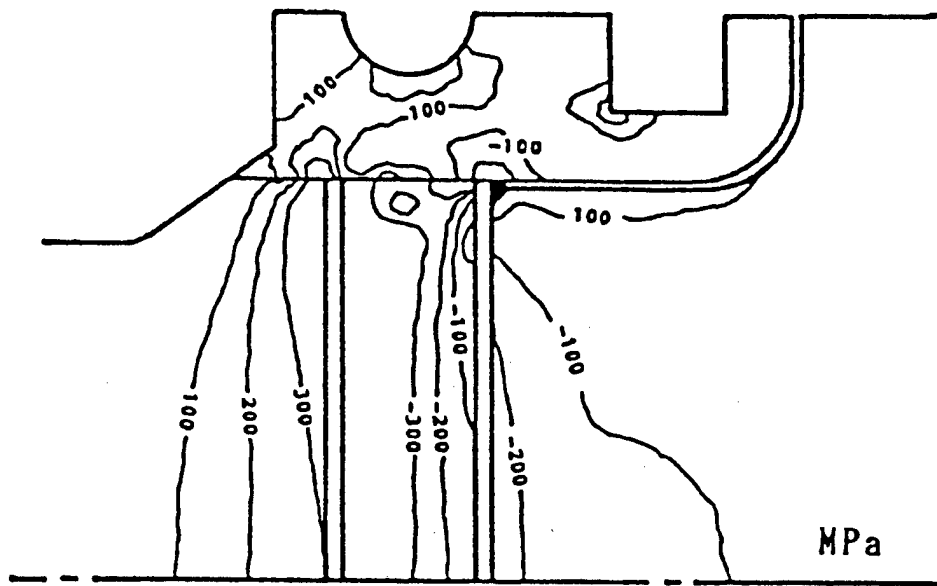


Figure 5.1.2.4 Distribution of Residual Stresses at Bonded Sections

be expected of them, and as a result, a large stress in any single place in the component leads to catastrophic failure. Since the values of stresses are greatly affected by a variety of factors ranging from the external dynamic forces and the thermal stresses arising from temperature distribution to the concentrations of stresses as determined by the sizes, kinds and shapes of internal defects, the strength of a part is not determined by the load of stress working on it alone but is also affected by the distribution of microscopic defects. In consideration of the scatter of defects, the relatively simple Weibull statistics have conventionally been used. Although it has the advantage that a minimum number of parameters (two) enables an outline of the strength to be obtained, the technique is far short of truly guaranteeing quality. This section describes the current state of the design reliability and materials science centered in the development of turbochargers.

(a) Catastrophic failure strength of rotation and design reliability

This section describes the catastrophic failure strength of rotation and reliability in the design of ceramic turbochargers. Ceramic failure is caused by defects in the material and the failure strength is governed by the largest of the defects in the material, so there is a large dispersement of strengths. Consequently, the strength values are defined as statistical values, and they are usually expressed by the Weibull distribution function.

The ceramic rotor's strength was evaluated by using a gas rotation testing system that is rotated and driven by combustion gas, of which the number of rotations per minute of the rotor and the temperature of the gas flowing into the rotor can be freely set. Figure 5.1.2.5 shows the results obtained in the catastrophic failure strength of rotation test conducted using an actual rotor. The broken line shows estimates on the catastrophic failure strengths

of rotation, which were obtained first by calculating, using the aforementioned stress analysis results, the effective volume of the actual rotor, and then by feeding into the computer the strengths of testpieces cut out from the rotor and the effective volume of the rotor.

(b) Fatigue life and design reliability

While in operation, a turbocharger rotor is subjected to thermal stresses because it is exposed to centrifugal stresses arising from its rotation and high-temperature exhaust gases. Ceramic fatigue indicates a phenomenon in which an initial crack in a rotor grows under the stress working on it and subsequently leads to the rotor's failure when it reaches a critical length. Hence, the time needed for a crack to grow from its initial length to its critical length is considered its fatigue life, and the fatigue life is determined by the initial length of the crack and the stress working on it. Life estimates, calculated with the element of fatigue factored in, can be obtained from the actual rotor's fatigue parameters and Weibull values, and an example is shown in Figure 5.1.2.6.

In practice, in order to guarantee the life requirements for a whole batch of products, ingenuity is needed to make sure that the initial crack is kept below some length so that it will not grow to its critical length. To that effect, the so-called surety tests have been conducted in which the stress calculated based on the maximum permissible defect length is applied to rotors and those that fail are removed. As shown in Figure 5.1.2.7, the failure rates for those rotors that have undergone surety tests have been confirmed to lie above the line of their minimum life estimates.

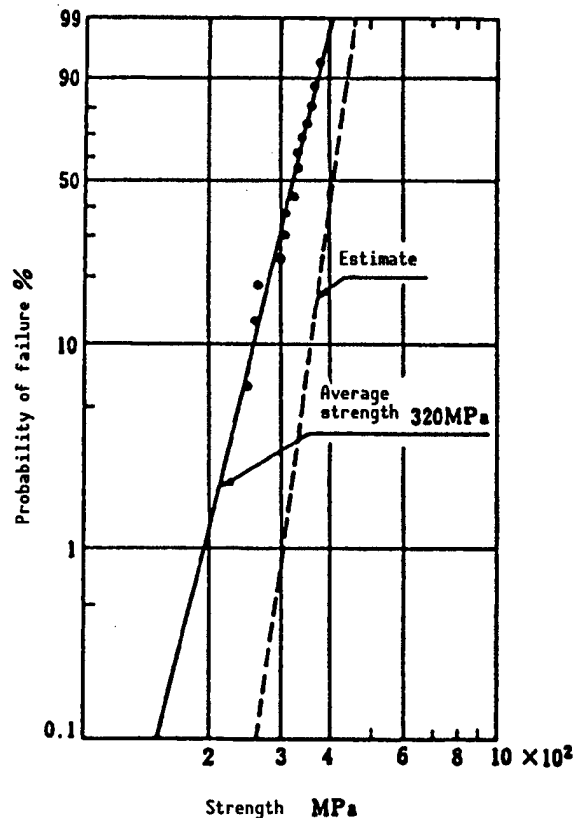


Figure 5.1.2.5 Catastrophic Failure Strength of Rotation in Actual Rotor

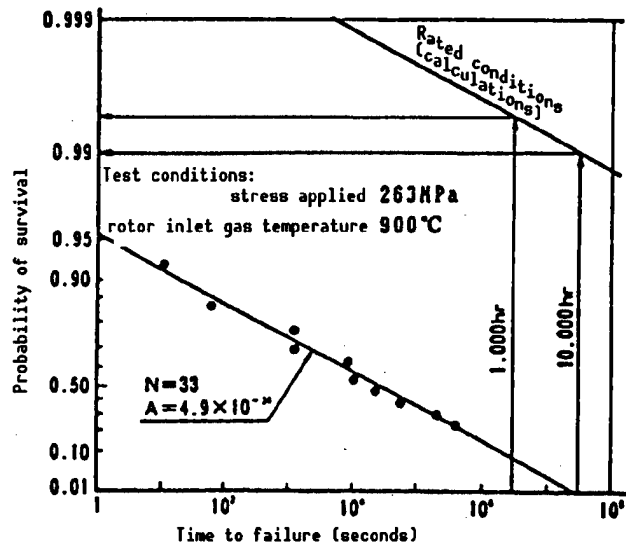


Figure 5.1.2.6 Fatigue Life and Probability of Failure in Turbocharger Rotor

(c) Collision strength and design reliability

In case foreign particles flying in from systems high above the turbo-charger hit the tips of rotor vanes on their negative pressure side at high velocities, the entire rotor itself may fail. Therefore, when designing parts that rotate at high speeds, their reliability must be designed taking into account the probability of their colliding with foreign matter. From the results of measurements of bending strengths which were taken after letting foreign particles bump into ceramic testpieces at high velocities, it is known that different ceramics have greatly different impact characteristics, as shown in Figure 5.1.2.8, so materials design must be conducted after taking into account their characteristics when hit by foreign matter. Relations between thickness of ceramics and their catastrophic failure were obtained using model testpieces, and the stresses that ensued when loads were applied locally to the rotor vanes' tips were analyzed. These efforts have brought a clue on how to increase the resistance of ceramics when hit by particles. Using an actual rotor, various collision scenarios were drawn up by changing the particles' points of impact on the vanes, the shapes of particles impinging on the vanes, their velocities and their volumes and material qualities, and reliability confirmation tests were conducted by using a test rotor.

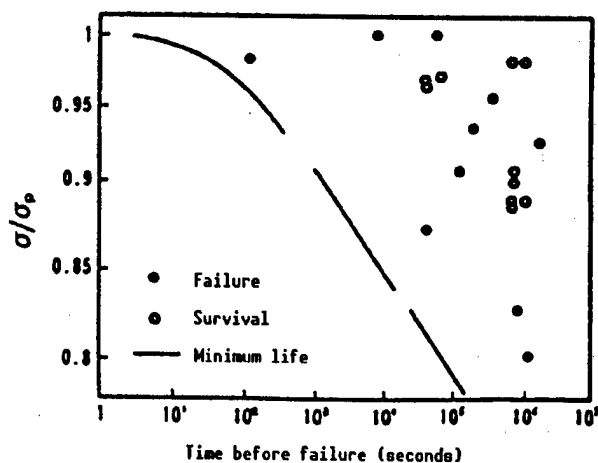


Figure 5.1.2.7 Fatigue Life After Surety Testing in Turbocharger Rotor

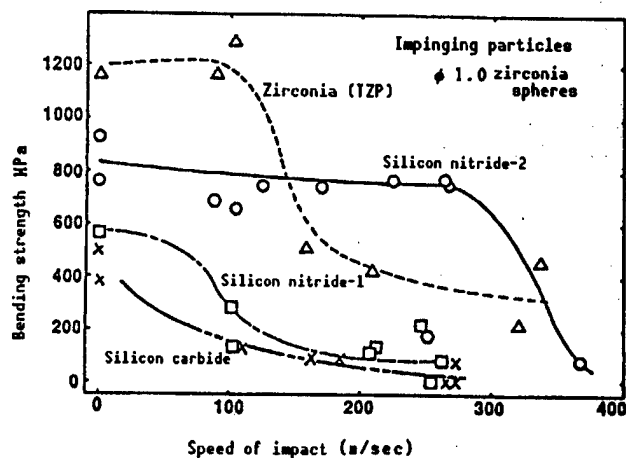


Figure 5.1.2.8 Relationship Between Speeds of Impact of Various Qualities of Materials and Bending Strengths

Thanks to these optimized efforts, as shown in figure 5.1.2.9, in the newly designed CNR-1 the critical weight of impact that causes it to fail when hit with the force is raised two times that for CN-1. These efforts, together with the efforts for coming up with optimal designs for all rotor systems that may generate foreign particles and for implementing thorough process controls, have produced high reliability of the product.

(4) Current State of Materials Science in the Manufacturing Process Design

When using ceramic parts in place of metal parts in engines, the designs of their shapes must be determined not only from consideration for performance and stress distribution but also from the perspective of the ease of manufacturing. Again, the manufacturing process must be designed in such a way that the advantages of ceramics not seen in metals can be put to the best use. Internal or surface defects in ceramic parts are generated in the manufacturing processes involving molding, sintering, and processing. As a result, finished ceramic parts usually have lower levels of strength than those of testpieces. Therefore, in order to improve the strength and reliability of ceramic components, the manufacturing processes themselves must be designed so that they will generate as few defects as possible. Again, if ceramics are to find increased applications, their cost must be reduced. In this respect, the manufacturing process of ceramics has room for improvement, if only to bring down the cost.

This section describes the current state of the manufacturing process and materials science of silicon nitride.

(a) Manufacturing process, strength and reliability

In using ceramics under high-stress conditions, the first consideration is that they have sufficient strength to withstand the environment in which they are used. The fracture strength (σ) of ceramics is expressed by the fracture toughness (K_{IC}) and the size of a crack in the material (a)

$$\sigma = K_{IC} / Y\sqrt{a}$$

where Y is the form factor of the crack. Therefore, factors governing strength can be broadly divided into the fracture toughness of the material and the crack caused by structural defects.

In examining the fracture surfaces of ceramics, flaws, such as surface scars, voids, coarse particles, and impurities, that ultimately led to their failure will be found. Figure 5.1.2.10 shows the relationship between fracture stress and defect size in ceramics of silicon nitride. As the defect size increases, strength decreases, but the relationship differs from one type of ceramic to another. This is because ceramics are brittle materials. A crack in a ceramic

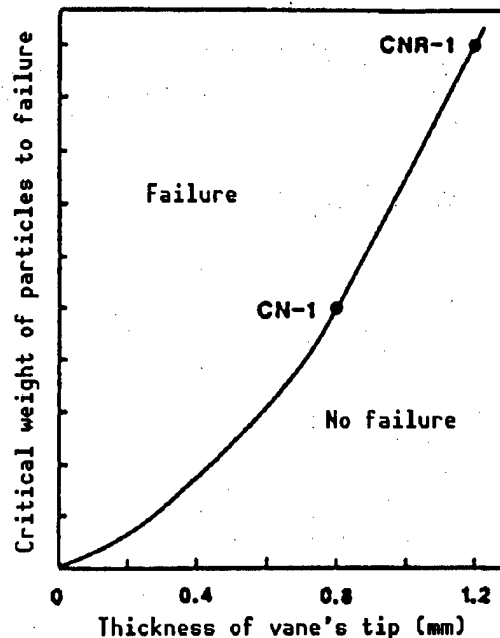


Figure 5.1.2.9 Relationship Between Thickness of Vane's Tip and Resistance to Impact by Particles

generated by a flaw in the material tends to lead to a concentration of stress in the area, which ultimately leads to the ceramic's fracture. The size of the crack differs depending on the type of flaw.

In most cases, the generation of defects can be traced back to the raw material powder and manufacturing process. As for the mechanically machined surfaces of ceramics, the defects are usually caused by grinding scars, and the defects in the interiors of sintered bodies are mostly represented as coarse particles and impurities. Voids are believed to be caused by the admixture of organic impurities like cotton dust and molding defects, coarse particles generated by the abnormal grain growth during the sintering process, and impurities introduced in the manufacturing process or contained in the raw material powder. As seen above, the causes for the generation of defects are numerous, but a widely used method to obtain high-strength sintered bodies is to probe the causes for failure and input the information into the manufacturing process as feedback.

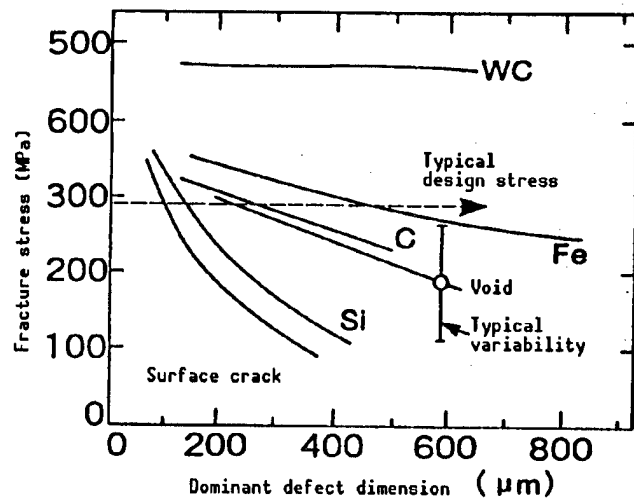


Figure 5.1.2.10 Manufacturing Defect and Strength of Sintered Body

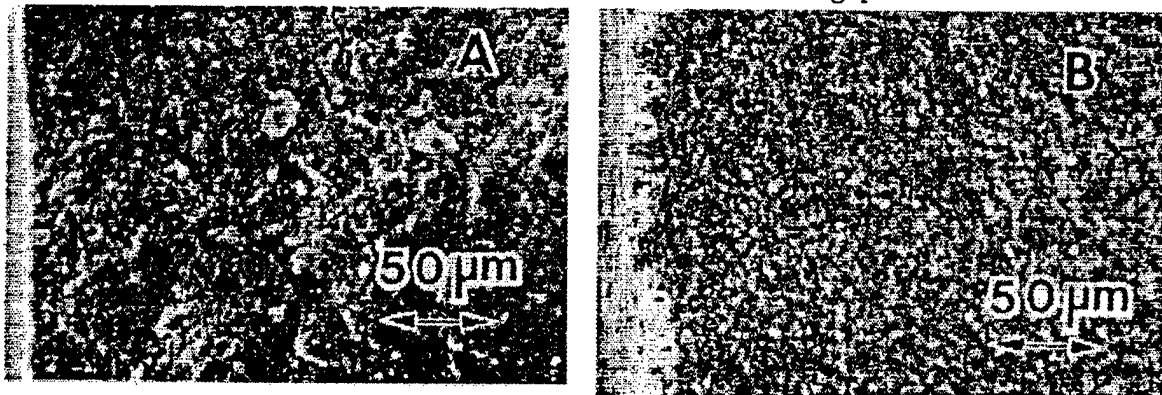


Figure 5.1.2.11 Voids Near Surface of SiN Sintered Bodies

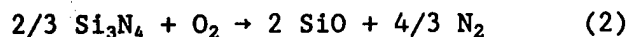
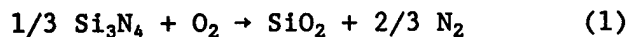
- (a) A sintered body obtained by subjecting silicon nitride to sintering at 1,700°C for 15 minutes under 2 MPa of nitrogen gas and then by raising the temperature to 70 MPa (gas pressure sintering)
- (b) A sintered body obtained by subjecting silicon nitride to sintering at 1,700°C for one hour under 0.1 MPa of nitrogen gas (normal pressure sintering)

Figure 5.1.2.11 shows an example in which an improvement on the sintering process has enabled voids near the surface to be reduced. In the case of the normal pressure sintering (B in the figure), a large number of small voids

were generated because silicon nitride and additive disintegrated near the surface of the sintered body during sintering, and the strength of the sintered body after grinding reached 774 MPa but the strength of the sintered body not receiving grinding dropped to 303 MPa. In the case of process (A), in which sintering was conducted first under 2 MPa of nitrogen gas and then the gas pressure was raised, the generation of voids in the sintered body was inhibited because disintegration of the silicon nitride and additives was suppressed by the high gas pressures, and the sintered body maintained a strength of 652 MPa even before grinding.

(b) Materials science of sintering additives for silicon nitride

Since silicon nitride is a material of high covalence, a dense sintered body of the material can usually be obtained by means of a mechanism in which some oxide additive is added to the compound to produce a liquid phase and the mixture is sintered. The sintering additive is usually determined by a trial and error process, but introduced below is an example of screening in which the selection of some suitable additive is conducted using thermodynamic data. In this process, the approach to screening is to eliminate oxides that cause unfavorable reactions to occur when sintering silicon nitride at its sintering temperatures. The reactions are considered below:



For ensuring that the silicon nitride will not be dissolved in a reaction of it with the oxide additive, the following conditions must be met:

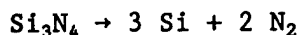
$$\Delta G_3 < \Delta G_1, \Delta G_2 \quad (5)$$

$$\Delta G_4 < \Delta G_1, \Delta G_2 \quad (6)$$

Figure 5.1.2.12 shows the results of the calculations. Oxides that have been reported effective in experiments are entered in the effective zone delineated by the oblique lines, and the technique allows for discovery of some new sintering additives.

(c) Materials science for sintering conditions of silicon nitride

When sintering silicon nitride, consideration must be given to the stability of the material at high temperature. Under high temperature conditions, silicon nitride undergoes the following reaction and is pyrolyzed.



The above reaction causes the silicon nitride to pyrolyze in 1 atm nitrogen gas at temperatures above 1,850°C, so there are upper limits to the sintering temperature at normal pressure. A gas pressure sintering process—a technique of sintering at high pressures in a medium of nitrogen gas—has been proposed as a method of making it possible to sinter silicon nitride at high temperatures while suppressing its pyrolysis. However, high nitrogen gas pressure is harmful to the final-phase sintering of silicon nitride. Consequently, the conditions for sintering silicon nitride are regulated by temperature and gas pressure and the optimal scope is proposed as a sintering map. Figure

5.1.2.13 shows the sintering map. In the figure, the following four temperature and pressure conditions are considered as the factors that determine the appropriate scope E.

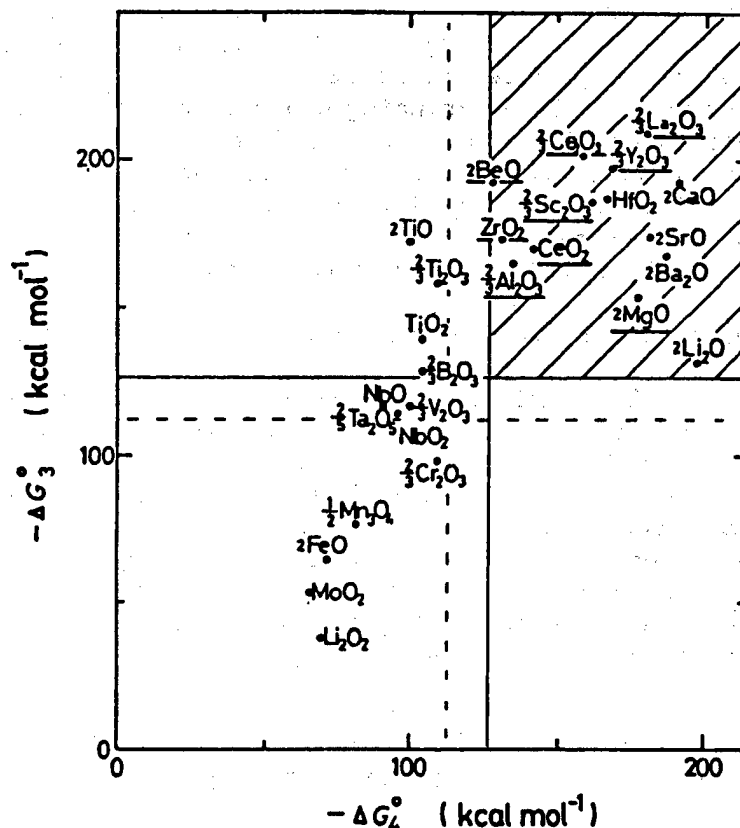


Figure 5.1.2.12 Thermodynamic Studies on Effectiveness of Additives to Sintering of Silicon Nitride

1) Minimum temperature-I (line 1 in the figure): A temperature at which the liquid phase that accelerates sintering appears, it shows the minimum temperature at which liquid phase sintering progresses. Therefore, densification does not progress at temperatures below the minimum temperature.

2) Maximum pressure (line 2 in the figure): This is the temperature at which the final-stage sintering is inhibited because of the high-pressure gas trapped inside the sealed pores, and full densification does not progress at pressures higher than the maximum pressure.

3) Maximum temperature (line 3 in the figure): A temperature at which the raw material powder silicon nitride begins to pyrolyze, the maximum temperature rises with increasing nitrogen gas pressure. At temperatures above the maximum temperature, no compact sintered bodies can be obtained because of the dissociation reaction.

4) Minimum temperature-II (line 4 in the figure): Line 5 shows the temperatures at which SiO gas is generated profusely because of reactions between silicon nitride and oxides in the starting raw material (silica and oxides as sintering additives). The minimum temperature rises with an increasing nitrogen gas pressure and the pyrolysis occurs vigorously at temperatures above the minimum temperature. Once pyrolysis reactions occur, the temperature at which the liquid phase is generated (line 1) goes up because of changes in the composition. Since the pyrolysis progresses more vigorously with a decreasing nitrogen gas pressure, the temperature at which the liquid phase is generated goes up with decreasing pressure.

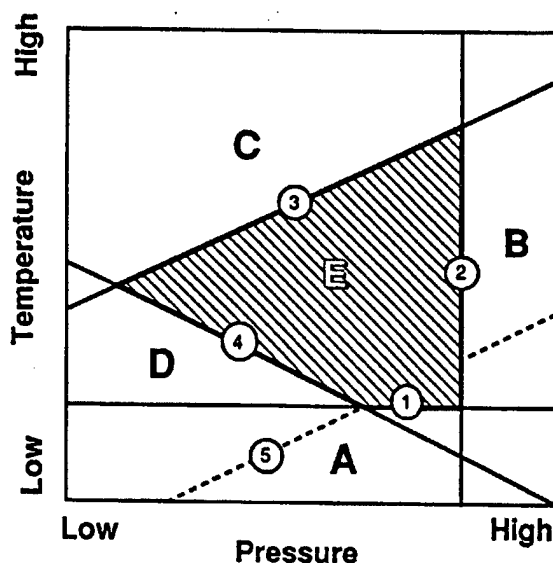


Figure 5.1.2.13 Sintering Map for Silicon Nitride

From the foregoing considerations, compact sintered bodies can be obtained in the domain E that meets the conditions in (1) through (4).

(d) Conclusion and prospects

About 10 years have passed since ceramics were initially used as structural materials for engines, and they are gradually finding increasing applications. However, if ceramics are to be used in a still expanded range of applications, improvements must be made in the design, reliability, and manufacturing process of ceramic parts, so that their performance will be raised, their cost reduced, and their reliability increased.

In the design of parts, an example is given using a technique of finite element analysis, mechanical stresses and thermal stresses to come up with a suitable part shape. In the design of the bonding mechanism, an example is given, in which residual stresses arising from bonding of discrete materials are reduced through calculations and experimentation.

As for the design reliability, examples of how to forecast catastrophic failure and fatigue failure of turbocharger rotors are given in experimentation and theory. An example is also given as to how to improve the strength to withstand a collision with a foreign object.

Regarding the design of the manufacturing process, the relationship between the manufacturing process and strength and reliability, and a materials scientific approach to sintering additives to silicon nitride and sintering conditions are described.

As a whole, as the ceramic technology stands now, little of the materials science theory or computer simulation is used in the development of ceramic products and much of the work is based on experience. However, if ceramics are to achieve further improvements in terms of performance, cost, and reliability and find still increased applications, a scientific approach must be adopted to the development of ceramic products.

5.1.3 Strength of Materials and Parts and Their Reliability

(1) Introduction

Development of structural ceramic materials and studies on their strength were begun several decades ago and the commercial applications of ceramic-based automobile parts started about 10 years ago. For years, ceramic engine parts have increasingly been mass produced. It is expected that a dramatic increase in the use of ceramics will take place centered on automobiles. It is because optional applications of ceramics, the materials having excellent mechanical and thermal features, for example, in those engine components where their features can be exploited to the highest degrees will greatly contribute not only to savings in energy and resources but also to the efforts for solving environmental problems. Materials and components development efforts have conventionally relied on a technique in which the trial manufacture and evaluation cycle is repeated in order to gain the experience needed to achieve the goal. Consequently, it will be highly meaningful to make efforts to sort out the accumulation of vast amounts of experience and turn it into a database in a bid to systematize or formularize those data while introducing theoretical methods based on materials science, since such an effort will be reflected as a gain not only in the speed but also the depth of research and development of ceramic materials and components.

From the perspective of material strength of ceramics, this section introduces the current state of applications of materials science techniques in the research and development of materials and components, brings to attention the inherent problems, and tries to explore the directions of future research and development.

(2) Current State of Use of Ceramics in Automobile Components

Figure 5.1.3.1 shows a whole picture of ceramic parts as candidates for use in reciprocating engines. Figure 5.1.3.2 [not reproduced], on the other hand, shows representative ceramic components. Research and development of ceramics has until now been focused on how best the various features of ceramics such as high heat insulation, high heat resistance, high

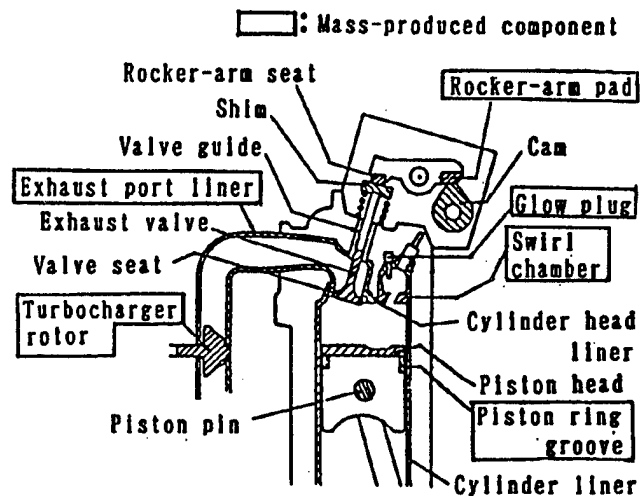


Figure 5.1.3.1 Candidates for Ceramic Parts in Reciprocating Engines

abrasion resistance, and light weight can be exploited to solve the important technique tasks for automobiles—high fuel efficiency, low pollution, compatibility with new energy resources. As things stand now, the number of ceramic components in engines is limited, but when the future for materials is concerned, it will not be an exaggeration to say that ceramics application technology is emerging as a key technology to solve the aforementioned technical tasks.

Figure 5.1.3.3 shows a thematic diagram of tasks that will have to be overcome if ceramics are to find adrastrically expanded range of applications. If ceramic parts are to become viable as commercial products, the basic principle is that they will have to be superb in terms of performance vs. cost

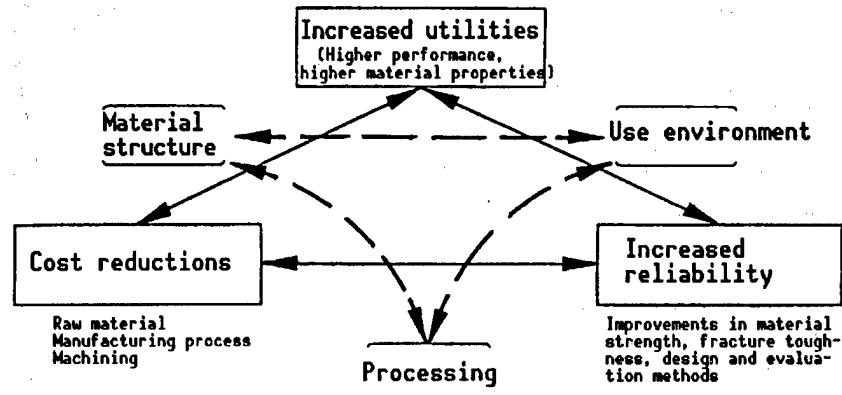


Figure 5.1.3.3 Tasks for a Gigantic Expansion in Applications of Structural Ceramic Components

and still retain a firmly established reputation in their reliability. As for strength and reliability, the issue centers on how to develop a ceramic component that has an ample margin of safety even under rigorous conditions of use. Expanding utilities of a ceramic component demands that engineers make increased efforts if only to guarantee strength and reliability under the designated use environment, and this in turn demands that more effort be made to improve the material strength and the design and evaluation methods. The key lies in whether or not one succeeds in raising the efficiency of the cycle of research and development or in narrowing the target of research and development by expanding the application of the scientific methods that are supported by the accumulation of experience obtained to date and by using extensively computer simulations, or by accelerating the growth of the technology still further.

(3) Current State of Scientific Approaches to Development of Materials and Components

(a) Material strength and fracture

Since structural ceramics are expected to have, among others, strong mechanical strength at high temperature, behaviors of fracture strengths of ceramics are schematically shown in Figure 5.1.3.4. The catastrophic fracture strength and the stress time or stress cycle dependent fracture (delayed fracture strength, fatigue strength) are further affected by the state of the environment, especially by microscopic behaviors of various materials under a corrosive environment.

Estimated strengths of ceramics obtained based on Griffith's theory, which may be called a macroscopic estimation of fracture, are generally larger than the experimental values obtained from actual materials tests by several orders of magnitude. This is because ceramic structures are made up of a large number of crystals but the formula of estimation does not necessarily take into account the

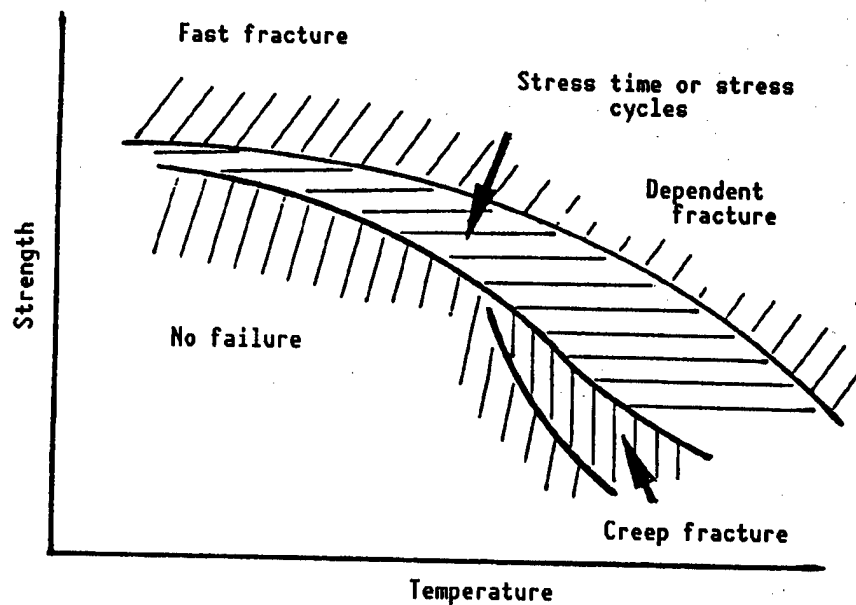


Figure 5.1.3.4 Strength-Temperature Diagram With Fracture Modes

microscopic state of material such as the relative relationship between crystals, the state of various inherent defects, the morphology of grain boundaries, etc. However, as for the ideal strength of perfect °C structures (single crystals), the estimated value and the experimental value are known to agree relatively well. Here, the ideal strength is a fracture stress of a ceramic having no defect or crack. Assuming the interaction between atoms comprising the ceramic is given by the sine function, then the ideal strength σ_{id} can be obtained from the following equation.

$$\sigma_{id} = \sqrt{\gamma_i \cdot E/\gamma_0} \quad (1)$$

where γ_i : is the surface energy of ceramic,
 E : is the modulus of elasticity of ceramic, and
 γ_0 : is the nearest distance between atoms.

γ_i and Δ_0 in equation (1) cannot be treated as experimentally clearly defined values, and given the fact that the above assumptions are far from the reality of materials, the estimated strength values of ceramics obtained from the above equation and the actual values obtained in experiments are far apart by several orders of magnitude. Hence, equation (2) has been devised to estimate the ideal strength by using values that can be clearly measured. From the standpoint of a single-phase theory, in this equation the approach is to correlate the ideal strength of ceramics with their melting point and the ideal strength of a ceramic is inferred from its various thermal properties.

$$\sigma_{id} \geq 3\bar{\alpha} \times T \times \bar{E}/(1 - 2\bar{\mu}) \quad (2)$$

(X = m, b, Tr)

where $\bar{\alpha}$: is the average thermal expansion coefficient,
 T_m : is the melting point,
 T_d : is the decomposition point,
 \bar{E} : is the average modulus of elasticity, and
 $\bar{\mu}$: is the average Poisson ratio.

Experimentally obtained strengths of whiskers and their estimated strengths obtained from equation (2) are shown in Table 5.1.3.1 for comparison. The two kinds of values for the covalent compounds SiC and Si₃N₄ relatively agree. However, this is the case only when the strength of perfect single crystals is concerned. The ideal strength can hardly be obtained for polycrystallines which are an aggregate of various crystals containing a substance which has a different composition from the grain boundary, some crystalline, or some amorphous sintering auxiliary elements.

Table 5.1.3.1 Comparing Theoretical Strength Values and Experimental Strength Values in Whiskers

Property Material	$\bar{\alpha} (\times 10^{-6} / ^\circ\text{C})(\neq 1)$ ($T_1 \sim T_2$) (°K)	μ	E (CPa)	T_m, T or T_{TR} (K)	ϵ_i	σ_{14} (CPa)	σ_i (Experi- (CPa)mental value)
SiC	4.3 (297-1144)	0.17	469	2,255 (Dissoc.)	0.04	20.7	20.7
Si ₃ N ₄	3.31 (294-1588)	0.22	299	2,144 (Decomp.)	0.04	11.4	13.8
B ₄ C	4.3 (297-1144)	0.19	362	2,700	0.06	20.3	13.8
Si	3.7 (373-873)	0.27	129	1,688	0.04	5.3	3.8
BeO	7.38 (294-700)	0.38	390	2,843	0.26	102.3	13.1
SiO ₂	12 (298-673)	(0.25)	117	(1,143) (846)	0.08 0.06	9.6 7.1	4.1
Al ₂ O ₃	9.6 (293-1800)	0.23	445	2,327	0.12	55.2	20.7
c-ZrO ₂	7.5 (299-700)	0.28	140	3,037	0.15	21.2	4.1
MgO	11.6 (294-811)	0.28	386	3,098	0.25	94.7	24.1
Mullite	4.9 (-)	(0.25)	220	2,103	0.06	13.6	-
NaCl	40 (-)	0.16	57	1,073	0.19	10.8	-

Figure 5.1.3.5 shows the static strength S of an Si₃N₄ sintered body at normal temperature and at high temperature in relation to the inherent defect size. When the defect size is relatively large (above about 50 μm), equation (3) having linear fracture dynamics is valid but it is not applicable in small defect domains.

$$S = K_{IC} / Y\sqrt{ae}$$

(3)

where K_{IC} : is the fracture strength at mode I,
 ae : is the equivalent crack length, and
 Y : is the coefficient.

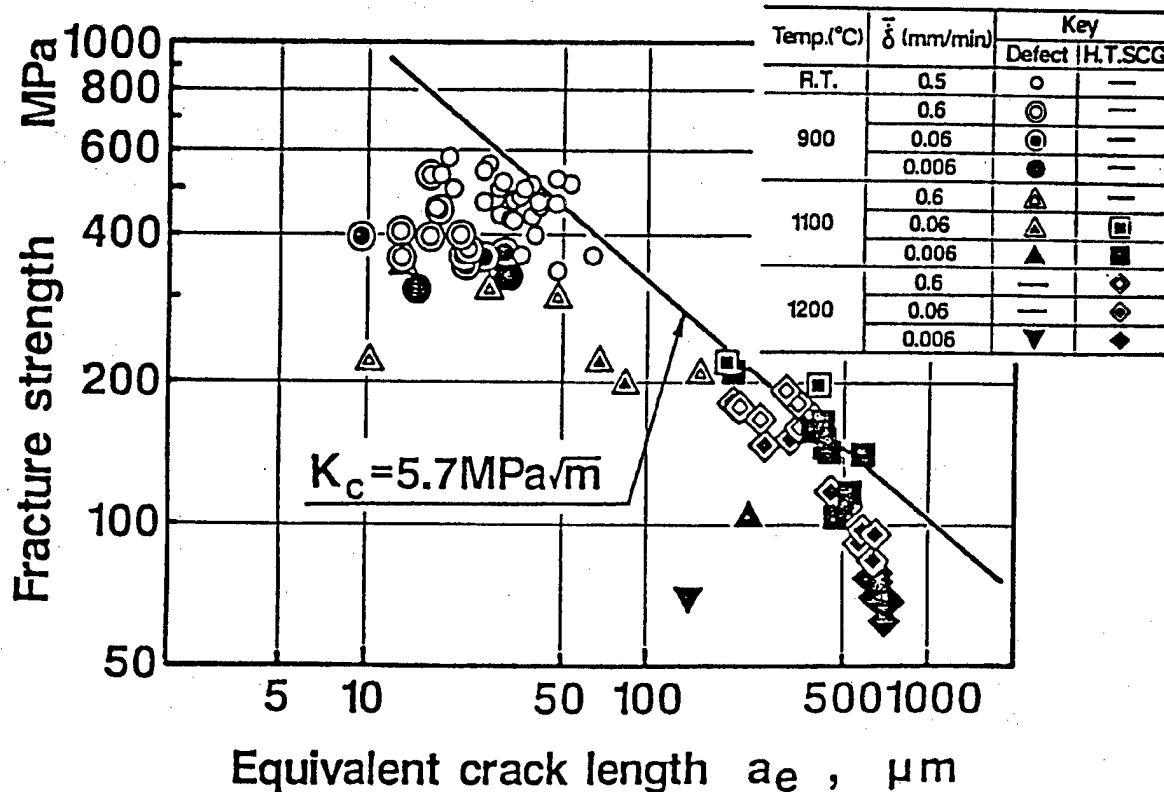


Figure 5.1.3.5 Relationship Between Tensile Strength and Crack Length

Many studies are presently being conducted to clarify the fracture behavior in this domain, but from the engineering or practical perspective, equation (4) has been proposed for estimating the strength of sintered bodies with microscopic defects. When the sizes of crystals in the domain at the tip of a crack are taken into account, equation (4) and the experimental results are known to agree well.

$$K_c / K_{IC} = \sqrt{1 + r / 2ae} / (1 + r / ae) \quad (4)$$

where K_c : is the critical stress intensity factor,
 ae : is the equivalent crack length;
 r : is the crystal grain diameter at the crack tip ($r=6d$), and
 d : is the average crystal grain diameter,

Figure 5.1.3.6 shows the K_c / K_{IC} ratio as a function of the ae/d , that is, the ratio of the size of various defects, such as voids, inclusions, and artificial defects, to the crystal grain diameter, in Si_3N_4 . Results in the

figure were obtained using equation (4) and they are in good agreement with experimental values. The use of equations (3) and (4) enables one to estimate relatively easily the strength of Si_3N_4 sintered bodies containing defects, and they are a valuable tool when designing or evaluating the strength of actual ceramic components.

In the course of component development, one often finds out that the strength of the specimen of a material and the strength of a part made from the material (a specimen cut out from the part) are different. The root cause for the different strengths is that the two are produced by different manufacturing processes, and the difference in strength arises from the fact that the two specimens have different microstructures, especially the state of coagulations of crystals, and that the defects contained in those microstructures are different. In parts with complex shapes, a slight localized change in the temperature condition during sintering, for example, could lead to changed microstructures in that area of the sintered body, thereby failing to impart the part the desired strength. Figure 5.1.3.7 shows the relationships between the strength, microstructure and sintering temperature in Si_3N_4 sintered bodies. The figure will enable one to understand well the foregoing descriptions.

Figure 5.1.3.8 shows a case in which the strength of specimen material and the parts' strength at high temperature are pretty much the same. This was realized because microstructures, especially the state of grain boundaries more close to the original goal aimed for in both the specimen and the parts.

Figure 5.1.3.9 shows the stress time and repeated stress-dependent (static fatigue strength, repeated fatigue strength) strength in Si_3N_4 . Ceramics also show the phenomenon of fatigue and this is caused by drops in their strength as a result of microscopic crack growth caused by microscopic defects or newly generated cracks. Consequently, getting an understanding of the crack propagation behavior under various use environments such as temperature is very important regarding the strength and life design of a component.

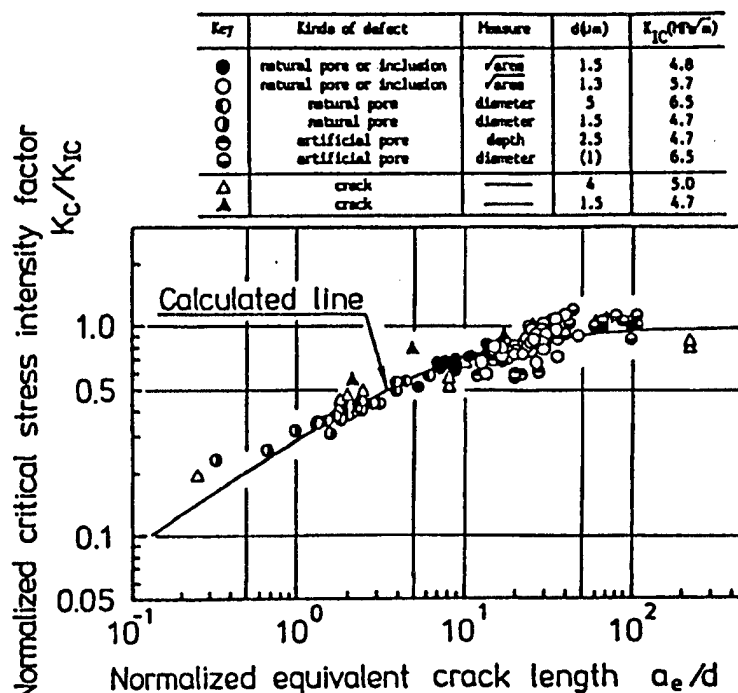


Figure 5.1.3.6 Relationship Between Crack Length and Fracture Toughness Ratio in Si_3N_4

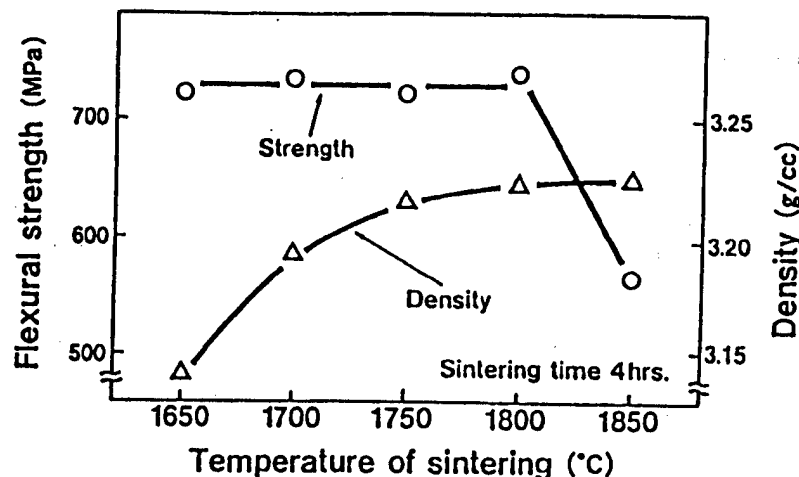
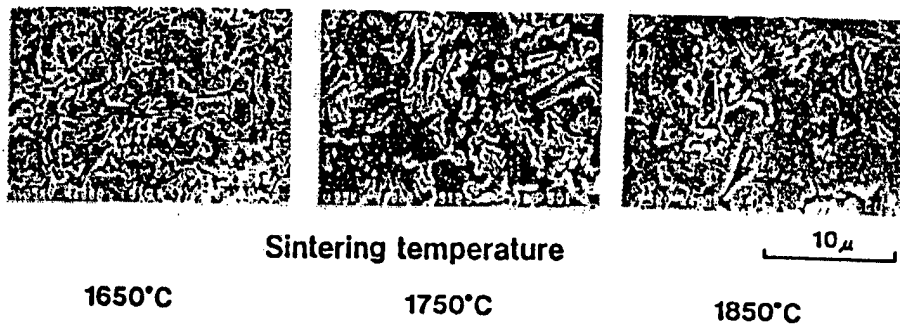


Figure 5.1.3.7 Relationship Between Strength, Micro-structure and Sintering Temperature in Si_3N_4

Figure 5.1.3.10 shows the behaviors of crack propagation in Si_3N_4 under various stress conditions. When a comparison is made of the same stress expansion coefficient, the crack growth speed da/dt in static fatigue (stress ratio $R = 1.0$) is smaller than the da/dt for $R = 0.1$. Also, da/dt for $R = 0.1$ increases with increasing stress frequency.

In addition to the above experiment, analyses have been made of crack growth behaviors under various stress conditions, and all the experimental results are approximately equal to the values obtained from equation (5).

$$da/dt = A_1 K^n, A_2 \Delta K^n \quad (5)$$

where K : is the stress expansion coefficient (constant stress),
 ΔK : is the stress expansion coefficient (stress amplitude),
 A_1 and A_2 : are the constants, and
 n : is the crack propagation coefficient.

These factors are all indispensable in estimating the lifetimes of components, but at present it is impossible to obtain them theoretically. An empirical approach through repeated experiments and studies is the only recourse open to us today.

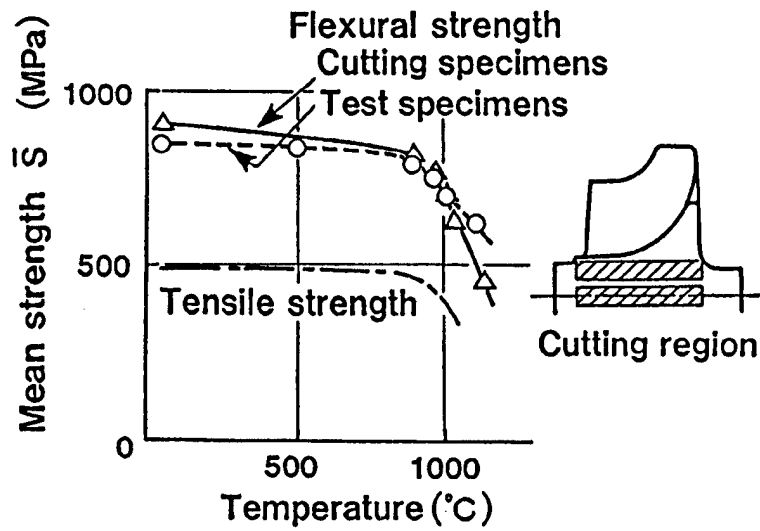
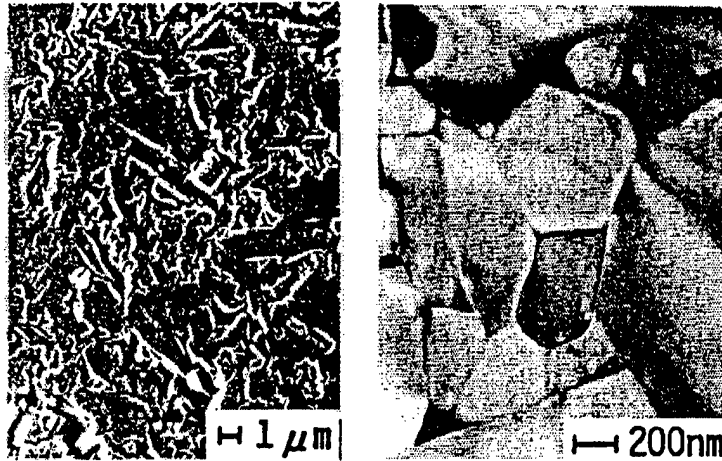


Figure 5.1.3.8 High-Temperature Strength and Microstructure in Si_3N_4

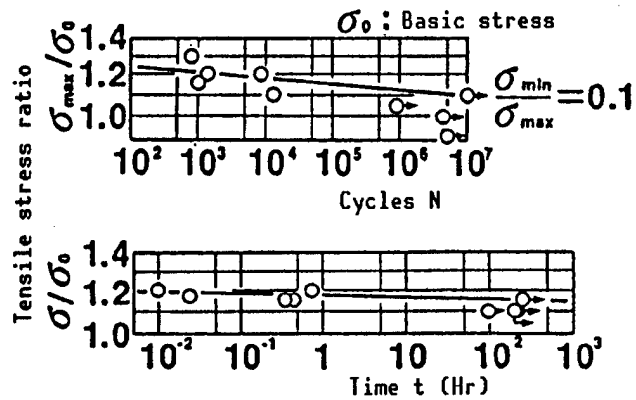


Figure 5.1.3.9 Fatigue Strength Diagram for Si_3N_4

Thanks to much research efforts, the mechanisms of fatigue of ceramics are being clarified. However, as the technology stands now, it is impossible to forecast the microstructures of a new material, while it is being designed, and have an estimate on the crack growth in it and to utilize the result in having simulations on the strength and life of a component made from the material. The only recourse available now is the empirical methods supported by experimental data.

(b) Strength and design reliability of commercial products and evaluation methods and proof tests

This section describes the applications of scientific methods to the strength and life design and evaluations of ceramic components for automobile engines.

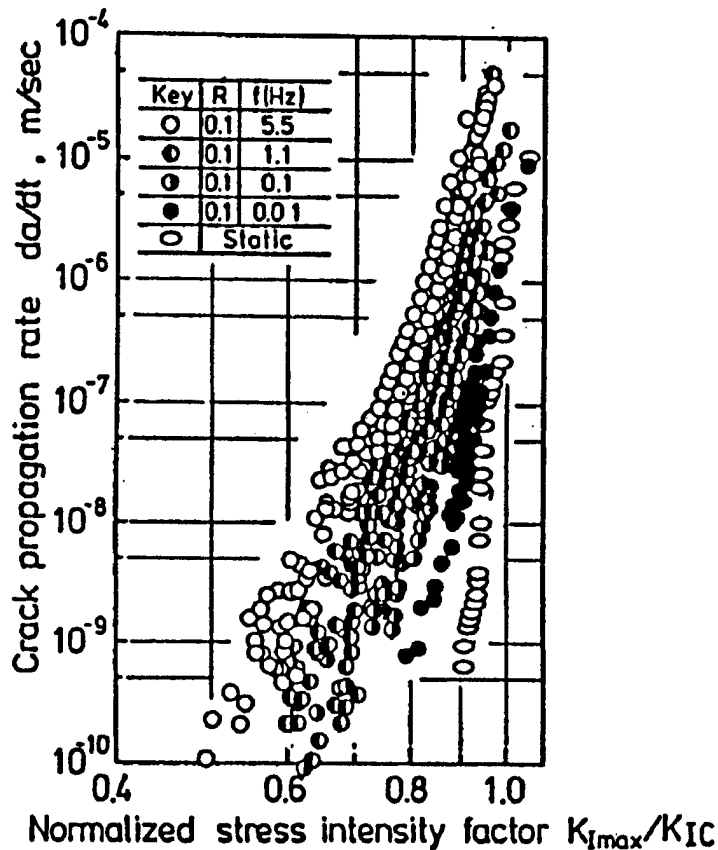


Figure 5.1.3.10 Crack Propagation Behavior in Si_3N_4

Figure 5.1.3.11 shows the basic flow of research and development of ceramic components. As for the analysis of material strength, the R&D flow can be broadly divided into the design and evaluation stages. The flow in R&D for simulating the strength and lifetime of components in the environment in which they will be put to service incorporated in engines consists of estimating the stresses working on a component, a process obtained by inputting the configuration of the component and the condition in which it will be put to service, of estimating the static strengths of local areas of the component, a process conducted by using the gained stress values and mechanical properties of the component's material, and of forecasting the fracture or life of the component when used in an actual engine.

Among the methods based on materials strength theories are the effective volume method, the stress-strength model, the linear fracture dynamics that is applicable to relatively large fractures, and the proof test method that is based on the probability theory and linear fracture dynamics. Figure 5.1.3.12 shows the mechanical and thermal properties required. Data on the material strengths used in simulations were obtained from empirical rules and experiments.

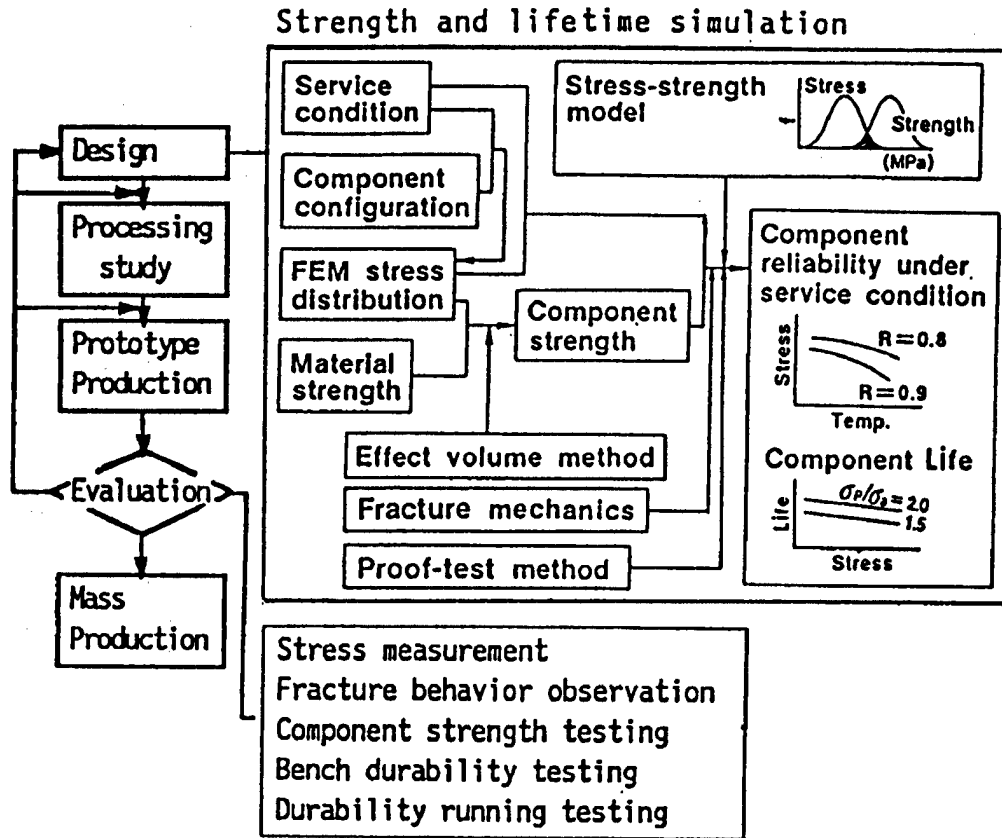


Figure 5.1.3.11 Basic Flow in R&D of Ceramic Components

The reliability R_i of a component with the initial strength = S_i is obtained from Equation (6), but if the stress load is σ_a , R_i can be obtained by substituting σ_a for S_i .

$$R_i = 1 - F_i = \exp \left[- \left(\frac{S_i}{S_0} \right)^m \cdot \int_V \left(\frac{\alpha}{\alpha_{\max}} \right)^m dV \right] \quad (6)$$

where S_0 : constant,
 α_{\max} : maximum stress,
 V : domain of the initiation of stress,
 F_i : fracture probability of S_i

Within the scope where the linear fracture dynamics is valid, the lifetime of a component under a constant stress σ_a can be calculated from equations (3) and (5).

$$t_0 = \frac{2S_i^{n-2}}{AY^2(n-2)K_{IC}^{n-2} \sigma_a^n} \quad (7)$$

Detecting various defects at the level of components by means of nondestructive testing technology has a limit, and the so-called proof tests must be conducted to ultimately assure the minimum strength and the minimum life of a

component. The life t of a component after undergoing the proof test is obtained from equation (8):

$$t = t_{\min} \left(\frac{S_p}{\sigma_p} \right)^{n-2} = t_{\min} \left(a + \frac{F_f}{F_p} \right)^{\frac{n-2}{m}} \quad (8)$$

where S_p : is the strength after proof testing,

σ_p : is the proof test stress,
 F_p : is the probability of fracture during proof testing, and
 F_f : is the probability of fracture of S_p .

Where there is no damage suffered in the proof testing, the minimum life after test is represented as t_{\min} and it is given by equation (9).

$$t_{\min} = \frac{2 (\sigma_p / \sigma_a)^{n-2}}{A Y^2 (n-2) K_{IC}^{n-2} \sigma_a^2} \quad (9)$$

When damage that may be inflicted during load releasing is taken into

account, the minimum value of strength after proof testing $S_{p \min}$ is given by equation (10).

$$\frac{S_{p \min}}{\sigma_p} = \left(1 - \frac{n-2}{n+1} \cdot \frac{\dot{\sigma}_{cr}}{\dot{\sigma}_u} \right)^{1/(n-2)} \quad (10)$$

where $\dot{\sigma}_{cr}$ means the critical unloading speed at which no damage is caused during unloading, and it is given by equation (11).

$$\dot{\sigma}_{cr} = \frac{A Y^2 K_{IC}^{n-2} \sigma_p^3}{2} \quad (11)$$

Seeking the dependency of $S_{p \min} / \sigma_p$ on $\dot{\sigma}_{cr} / \dot{\sigma}_u$, we obtain Figure 5.1.3.13. For example, when the unloading speed $\dot{\sigma}_u = \dot{\sigma}_{cr}$ and $n = 80$, damage equivalent to a 4 percent drop in the static strength is anticipated during the unloading process.

(c) Strength and life of turbocharger rotors

Figure 5.1.3.14 shows a simulation of stresses working on a turbocharger rotor. The FEM stress distribution has been plotted after taking into account the centrifugal forces by rotations and the thermal expansions brought about by temperature differences inside the rotor.

Mechanical properties

- Static strength
- Stress-time dependent strength
- Stress-cycles dependent strength
- Relation between strength and defect size
- Fracture toughness KIC
- Crack propagation behavior
- Oxidation and corrosion behavior
- Resistance for foreign object damage

Thermal properties

- Thermal conductivity
- Thermal diffusion coefficient
- Specific heat capacity
- Thermal expansion ratio

Figure 5.1.3.12 Mechanical and Thermal Properties Demanded of Ceramics When Used as Components in Engines

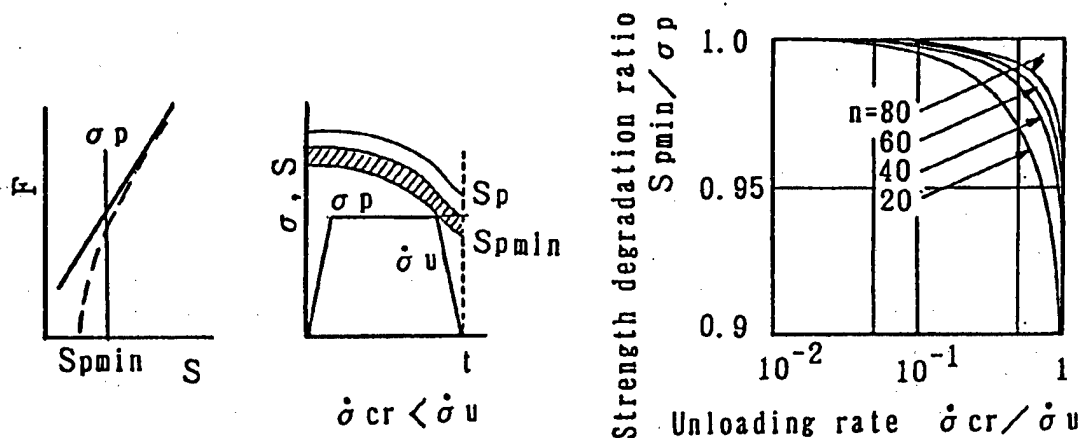


Figure 5.1.3.13 Strength Degradation Model During Proof Testing and Estimated Amounts of Damage From Proof Testing

It is necessary to confirm if the failure-prone segment identified in a simulation becomes the location of initiation of fracture under an overloading condition that is beyond realization in actuality, or if the estimated stress values agree with the actual stress values. According to the results of the estimation, the maximum stress is seen in axis R at the back of the rotor, and Figure 5.1.3.15 [not reproduced] shows a photograph of the moment of fracture obtained in an experiment conducted to confirm if fracture will actually occur at R when the rotor is rotating at excessively high rates. Cracks originating in the location are propagating in all directions, which agrees with the results of the simulation.

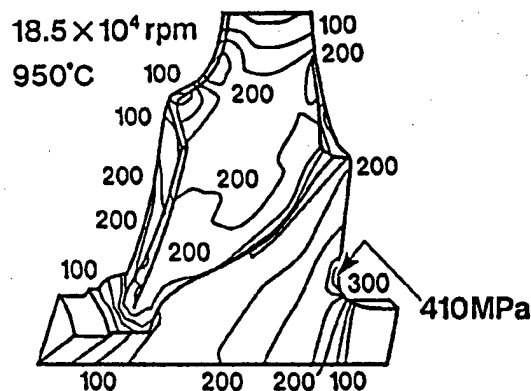


Figure 5.1.3.14 FEM Stress Distribution in Si_3N_4 Turbocharger Rotor

Since the rotor is rotating at high speed under a high-temperature environment, it is impossible to measure the stress working on it with the conventional methods. Therefore, as shown in Figure 5.1.3.16, a method of measuring stress has been devised, in which, assuming an artificial defect is generated in the location estimated to be subjected to loading of high stress, the stress is measured from the relationship between the defect size and the number of rotations that cause fracture. The application of a fracture mechanics method based on equations (3) and (4) enables the stress to be measured from the fracture rotation number.

When an assumption is made that the linear fracture dynamics is valid, from the crack propagation and behavior data in Figure 5.1.3.10, the results of the stress simulation in Figure 5.1.3.14 and the results of the measurement of the actual stress working on the rotor, estimated lifetimes of the segment of the

rotor subjected to loading of high stresses are calculated, which are plotted in Figure 5.1.3.17. The results can be used for the strength design in such cases as when one is trying to determine what level of proof test stress σ_p will need to be estimated against the applied stress σ_a if the rotor is to have the targeted design life and reliability.

(4) Tasks and Prospects

(a) Improvement of material properties and characteristics

The strength and life of a component is almost invariably determined by the local state of the component material. Furthermore, it may be said that the life of a component is almost invariably determined by the process of crack generation, or by the process of extension of microcracks caused by the crack and inherent defects. As described in equations (3) and (4), the strength of a component is determined by the fracture toughness of the component material. Also, from equations (7), (8), and (9), the initial-stage crack length (of a material) that is determined by its initial-stage strength and fracture toughness greatly affect the life of the component (made from it). Therefore, in the development of materials until now, the primary importance has been placed on how to overcome their brittleness and this will be the same in the future as well. Figure 5.1.3.18 shows the scatter of strength. Recently, attempts have been made to realize high-strength and high fracture toughness ceramics by controlling their microstructures, and in this respect, studies on Si_3N_4 material are making steady progress. In a bid to enhance fracture toughness of ceramics, active research is also being done on composite ceramics but here the difficulty is how to disperse different kinds of materials uniformly into the matrix.

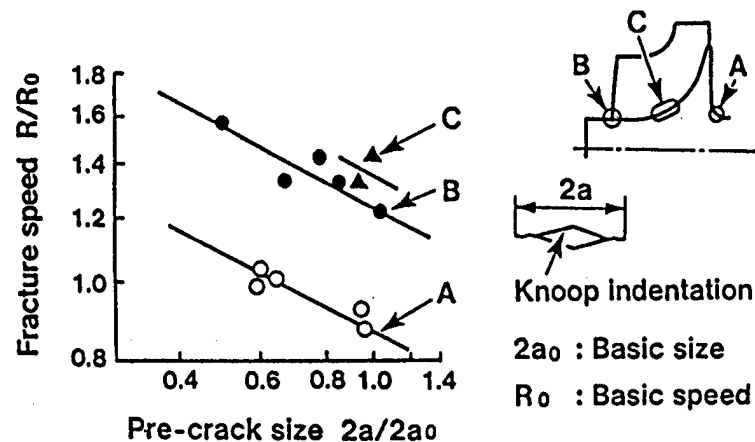


Figure 5.1.3.16 Relationship Between Artificial Crack Size and Fracture Rotation Number in Si_3N_4 Turbocharger Rotor

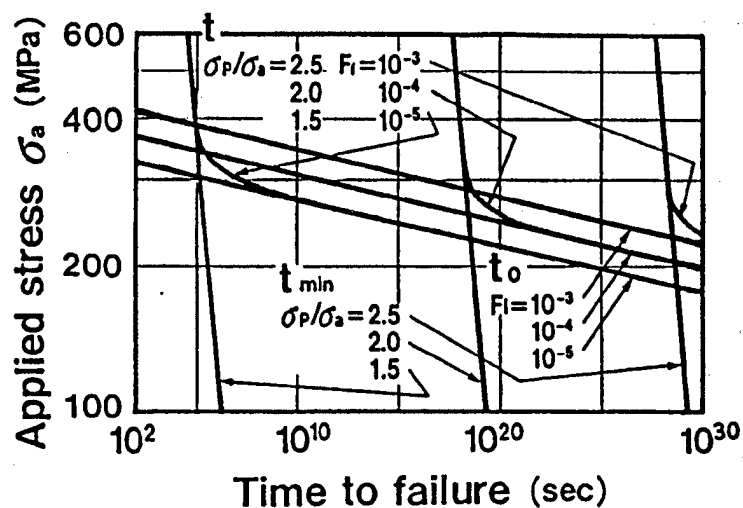


Figure 5.1.3.17 Estimated Life of Si_3N_4 Turbocharger Rotor

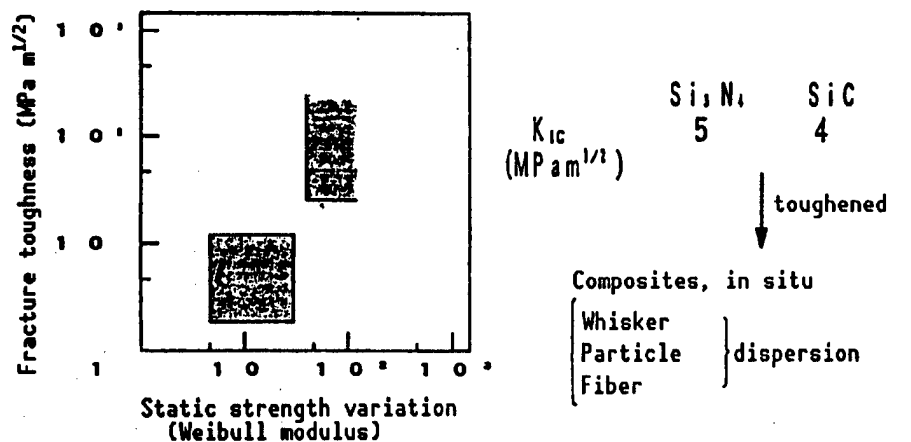


Figure 5.1.3.18 Fracture Toughness and Static Strength Variation in Structural Ceramics

In an in-situ type of approach, some attempts have been made to develop ceramic composites, in which the matrix itself is made of various different types of crystals. Figure 5.1.3.19 gives an example in which Al_2O_3 is reinforced with TiO_2 particles, and the technique is interesting in that it takes advantage of a dissolution and generation method.

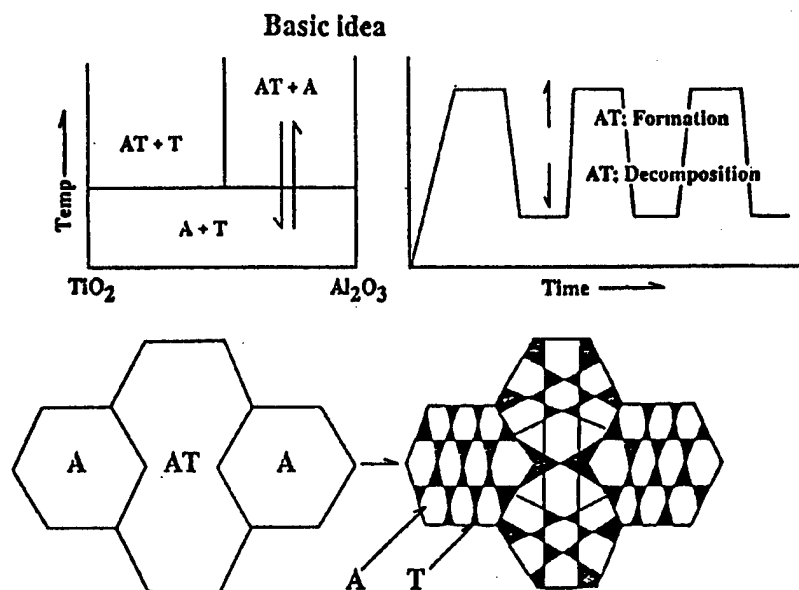


Figure 5.1.3.20 shows a schematic relation between static strength and crack size using the fracture toughness value as a parameter. Research on how to explain the fracture phenomenon of microcracks that cannot be explained by the linear fracture dynamics will take the place of key research in the development of materials featuring both high strength and high

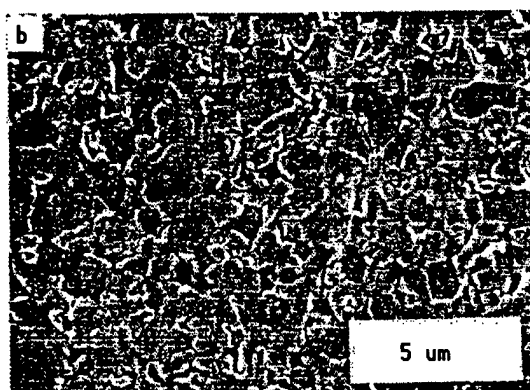


Figure 5.1.3.19 Microstructures of Al_2O_3 Reinforced With TiO_2 Particles Dispersed Inside, Prepared by Dissolution and Generation Method

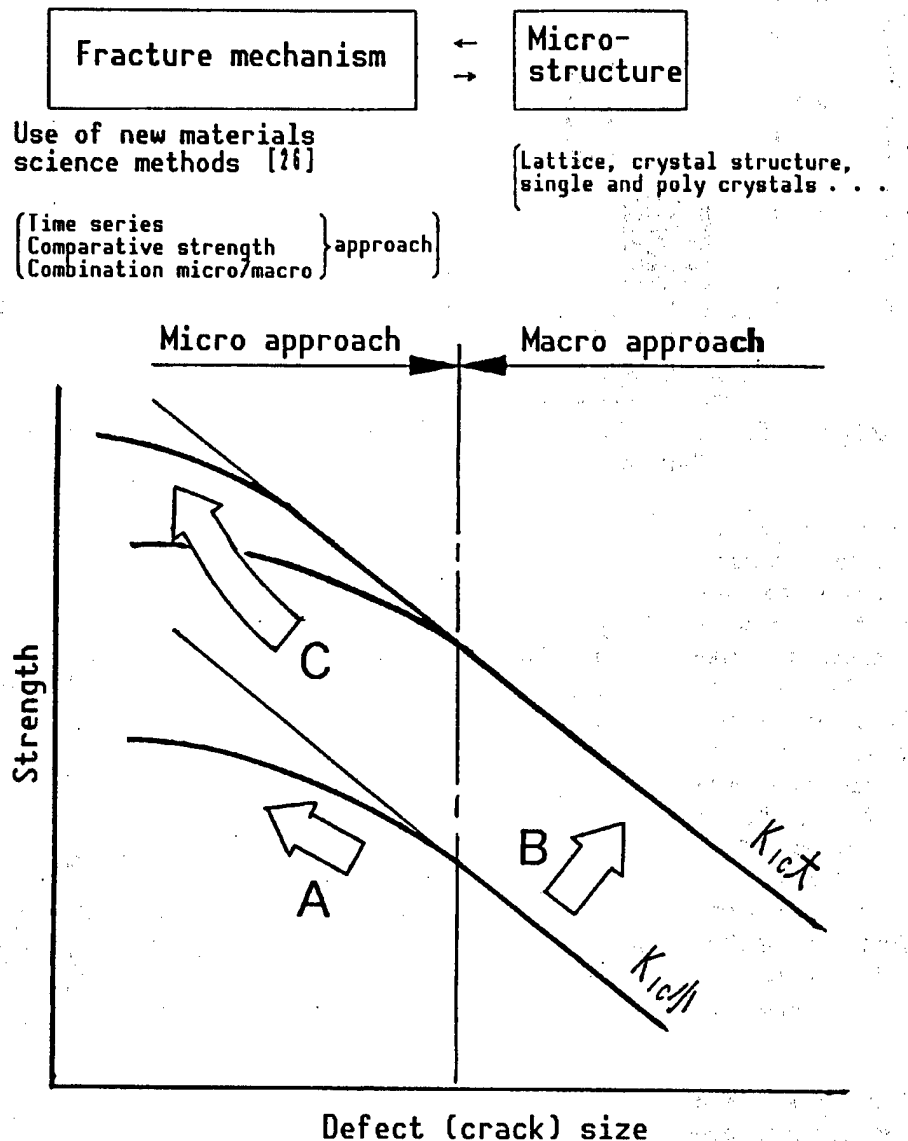


Figure 5.1.3.20 Domains Where Expectation Is Placed on Materials Science in Improving Strength of Ceramics

toughness. Research and development into the "C" direction, a mixture of direction "A" involving process refinement and direction "B" where the thrust is toward development of composite materials, will become extremely important.

A research project is being undertaken to clarify the mechanisms of fracture from various angles, such as a time series approach from the initial crack to the final fracture, the relative strength that transcends the framework of materials, and a combination microscopic and macroscopic approach. Great hope is placed on materials science theories and empirical rules that may result from the project.

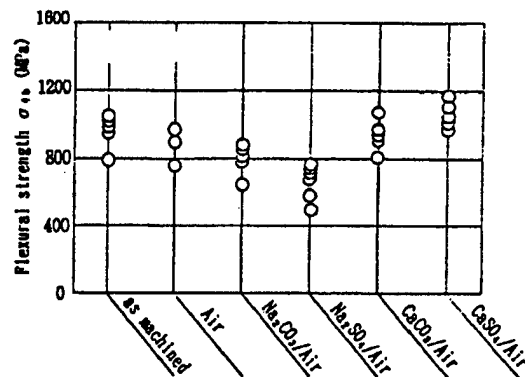
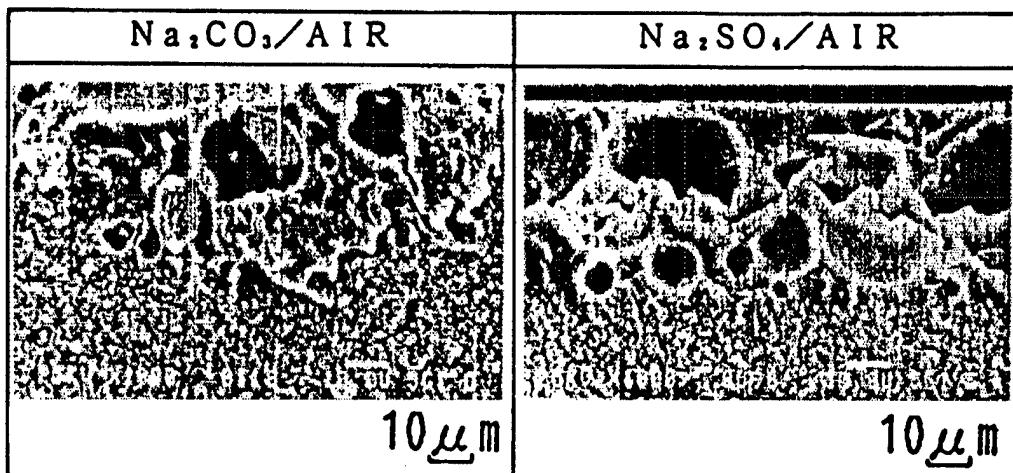


Figure 5.1.3.21 Bending Strength and Fracture Surface in Si_3N_4 After Corrosion at High Temperature

On the other hand, behaviors of materials under extreme service environments must be characterized. The service environment for the ceramic components in automobile engines, the targeted area of application of ceramics for now, is a combustion gas atmosphere of below $1,000^\circ\text{C}$. However, the service environment for gas-turbine engines of higher efficiency is said to reach a temperature of around $1,400^\circ\text{C}$. Figure 5.1.3.21 shows the bending strength and fracture surface in Si_3N_4 after corrosion at high temperature. The matrix, when deposited with carbonate or sulfate, is known to lose its strength even at temperatures of about $1,000^\circ\text{C}$, because the dissolution of Si_3N_4 leads to the generation of pores that trigger fracture. Since these molten salts are contained in small quantities in combustion gases from a turbine, the elucidation of the mechanisms of corrosion at high temperature and the development of high-corrosion-resistant materials are essential.

(b) For raising the efficiency of development of materials and components and for improving their strength and reliability

If there existed a material design expert system based on the established material strength theory and experimental and empirical rules, it would prove

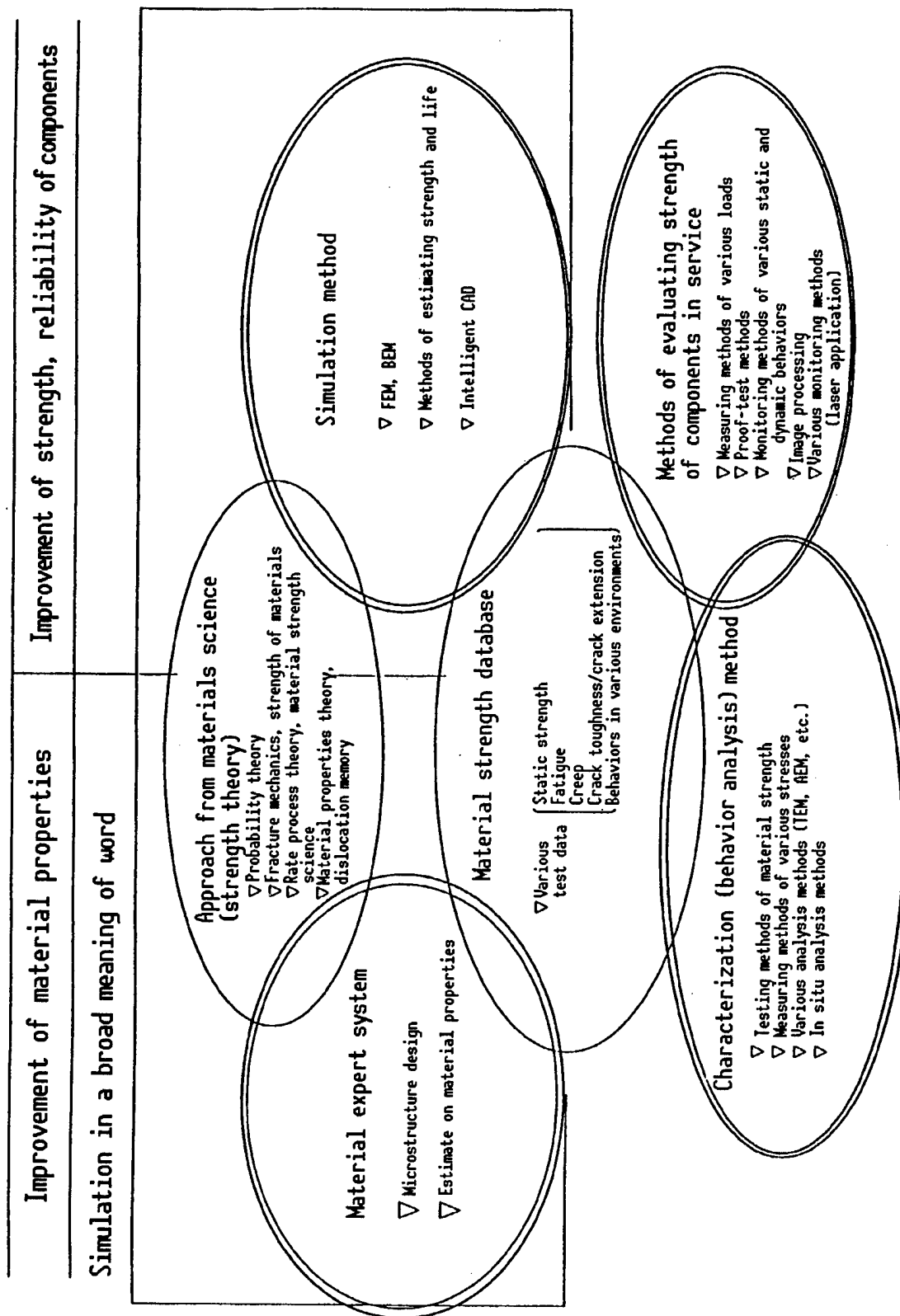


Figure 5.1.3.22 An Approach to the Strength Design and Analysis in Advanced Materials

to be a highly effective tool in enhancing the material properties and in increasing the strength and reliability of components, thereby facilitating the research and development of materials and components. The concept is given in Figure 5.1.3.22 illustrating the strength design and analysis of advanced materials. Once the day arrives when engineers are able to design the microstructures of materials and forecast their properties in the course of their routine research and development activity, ceramics will prove to be a catalyst for technological innovations.

Table 5.1.3.2 Idea for Microstructure Design and Material Properties Forecasting Expert System (Material strength and reliability)

1. Goals	(1) Controlling the properties of materials by controlling their microstructures. (2) Realizing simultaneously the two elements of increased material strength and heightened fracture toughness. (3) Formulating existing materials science methods into systems of science and their application (probability theory, fracture mechanics, rate process theory, various characterization methods).
2. Tasks awaiting solution	(1) Correlation between microscopic and macroscopic mechanisms in fracture behavior. (2) Correlation between material and process and fracture behavior. (3) An experimental approach to the pursuit of fracture behavior Theory = Empirical rule
3. Expectations	(1) Serendipity that allows anyone to take an interdisciplinary/inter-industry approach. (2) A shorter development period and an increase in the sophistication of the development activity. (3) Creation of new materials.

The goals and tasks of an expert system are summarized in Table 5.1.3.2. Gaining still larger amounts of theoretical and empirical data on fracture behavior, described above, will further improve the utility of the expert system. A forecasting system of strength and fracture behavior of extremely high accuracy may not be hoped for, but as the system incorporates the currently available techniques in a variety of fields, it may enable us to have some insight into material properties. The system will no doubt impact the current trial-and-error approach to research and development, a practice based on a repetition of trials and experiments.

(5) Conclusion

The use of structural ceramics in practical applications has only just started. The research and development for exploiting the advantages of and correcting the disadvantages of ceramics will bring about not a small amount of innovation in machine systems and will no doubt contribute to society.

The history of research on the strength and fracture of ceramics is short when compared with that for metals. But, seen from the perspective of materials science, summing up whatever facts are known about ceramics at present and researching what should be done now to improve their properties objectively will be indispensable if solutions are to be found for their problems at the earliest possible date. Sorting out much of the R&D achievements by exploiting supercomputers and developing the expert system that will be able to show the direction of R&D may be said to be one of the most promising projects for now. However, if the system is to be successfully developed, in the field of research on the strength and fracture of materials, a stepped-up effort for an interdisciplinary approach will be needed.

7. Executive Summary

7.1 Summary of Survey Results

With respect to materials science of fine ceramics, a survey and study was conducted to analyze the current status of structural materials, functional materials, process technology, and composite technology, with an emphasis placed on the role of materials science of ceramics and its potential.

Today, fine ceramics are used in various applications, and the demand is to meet still advanced service conditions. One is the probe for and development of new materials that either show new functions or have drastically improved properties, and the other is the stable quality. For materials to be provided with stable quality, the following conditions must be met: precise control of the starting raw materials, optimization of the manufacturing process, an understanding of the phenomenon occurring in the manufacturing process of material; and an understanding of the correlation between the structure of a material and its functional properties. Materials science has a large role to play in each of the aforementioned areas, and its importance will increase in the future.

Conventionally, material development of ceramics has mainly relied on experiments, and the effectiveness of theories and calculations based on materials science has been limited to their use in confirming the results of the experiment. The lack of a technique to link controls of microscopic states to the manifestation of macroscopic functions in the field of ceramics by freely controlling the bonding of atoms and particles comprising material has been the major cause. Further, the biggest factor obstructing the establishment of ceramic materials science as an established science based on solid physics and solid chemistry has been the complexity of the forming process of ceramics and their complex structures including lattice defects and grain boundaries. Another factor is that although it is true that the more complex a structure a material has, the more effective an approach of analysis based on materials science should be, but researchers of solid physics and solid chemistry have been shunning ceramics because of the exceedingly great complexities of their structures. As discussed in Section 2, we are facing the intrinsic problems of materials science of ceramics in their use as structural materials and functional materials as well as in the technologies of processing them or making composites of them. However, as can be seen in the cases of research and development of oxide superconductors in recent years, participation of researchers of solid physics and solid chemistry in ceramics research is becoming more common. Further, measuring instruments that make it possible to clarify microscopic states of materials (electrons, atoms, and particles) have come to be used one after another in the research and development of ceramic materials, with the result that an accumulation of the atomic- and molecular-level information, a kind of information hardly to be expected until now, is advancing. For example, the transmission electron microscope (TEM) is making it possible to routinely observe the structures of grain boundaries of ceramics and structures of surfaces of bonds between ceramics and metals. It is now possible even to observe in situ the extension of linear defects in ceramics.

On the other hand, in the fields of solid physics and solid chemistry, the rapid advances in computers and the steady progress of theories are making it possible to conduct the kinds of calculations that were unavailable in the past, in various fields, and their potential is without bound. To be concrete, as described in Sections 3 and 4, methodologies of ceramics that are based on solid physics and solid chemistry, to include electron theory and macroscopic theory, are being readied. Steady progress is seen in the solid physics and solid chemistry-based ceramics science, such as the ability to calculate the grain boundary structures of ceramics by means of quantum mechanisms calculations based on electron theory and compare the results with TEM observations and the effective use of molecular dynamics in the probe for ceramics materials (Section 5). That is, a materials scientific approach (computational physics, computational chemistry) to ceramic materials is already beginning to take hold, and materials science, as computers keep on increasing in capacity, will be applied in various problems, contributing to the probe for new materials and the design of materials.

The basic problem in the material development of structural ceramics at present is the strength and fracture of the material and the component made from it. As described in paragraph 1 of Section 5, the difficulty of developing structural ceramics lies in the fact that the practical problem of evaluating the reliability of a material and a part made from it is directly linked to the hardest to explain of all the problems associated with materials science—strength and fracture. Discussing the highly macroscopic phenomenon called the phenomenon of fracture from a microscopic standpoint may be said to be premature, but it has already become possible to simulate the crack extension by means of the molecular dynamics and quantum chemical calculations based on the molecular orbital method have come to be employed in the case of fatigue fracture of glass. It will not be too long before these techniques, when used in combination with micromechanics, a phenomenon theory, will be able to forecast the reliability of materials and parts on the level of atoms. Further, the functional materials described in paragraph 2, Section 5, are the field where a ceramic materials scientific approach based on solid physics and solid chemistry is needed in place of the hitherto trial and error or carpet bombarding type of development. Almost all functional ceramics take advantage of the nature of electrons in material, and a quantum mechanics calculation method based on electron theory is indispensable in the probe for a new functional material or in the design of a material on the electron level. As described above, the possibility for such a technique is nearing reality.

Materials science is a science in which a complex phenomenon is analyzed in detail in order to extract the problems inherent in it. However, as is represented by the discoveries of oxide semiconductors, there are a large number of discoveries that have been made outside the scope of materials scientific forecasting. By analyzing examples of historic discoveries, it will be necessary to systematically promote development of methods for discovering new properties and new materials.

7.2 Plans for Projects

Based on the findings of this year's survey, the survey committee proposes the following plans for projects in order to promote and establish the materials science for ceramics and to establish the materials design systems.

(1) Theme: Research for the establishment of materials design technology for the ceramic system of materials and for the development of support systems for the technology.

(2) Project's Contents:

(a) Theoretical calculations from the microscopic level, explanation of various phenomena by simulations, and establishment of the materials design and forecasting technology

By subjecting ceramics-based materials to electron, atom, or particle level theoretical calculations such as the band calculation, the molecular orbital method, the molecular dynamics method, or the statistical dynamics method as well as to simulations, their various properties and their various phenomena will be explained from a microscopic level. Also, attempts will be made for designing and/or forecasting the properties and structures of materials. Emphasis will be placed on the comparison and study of the research results with the results obtained in microscopic experiments and observations. This will reveal the applicability and limits of the various theories and techniques, leading to the development of theories and techniques suited to materials. Development will be long-term and the experience obtained will be accumulated, in order to establish material design and forecasting technology. General-purpose software for various theoretical calculations and simulations will be developed, and a database will be compiled of microscopic parameters for the design and forecasting and the first principle calculation results.

Due to a quantum leap in the calculation means such as supercomputers and to the growth of various theories and calculation methods, in the material field of semiconductors, the techniques of explaining various phenomena from microscopic levels and of designing materials are reaching the stages of practical applications. In the field of ceramics, however, the attempts at establishing similar techniques have just begun and they are still limited to only a part of the field. In this project, research groups will be organized for each of the various phenomena or materials, or for each of the calculation methods, in order to systematically promote the explanation of theories and the establishment of the design and forecasting technology.

(b) Building a database to support the design of ceramics-based materials

To facilitate the work to design materials and forecast their properties, a database will be compiled that will contain information on a broad range of basic material properties such as thermodynamic data, phase equilibrium data, crystal structure data, diffusion data, and electric and magnetic data. A database will be compiled of various properties of ceramics-based materials

such as mechanical strength, toughness, fatigue characteristics, sintering characteristics, and various interfacial characteristics, to include data on the composition, microstructure, organization, raw material, manufacturing process and service environment. From the perspective of the design of materials, software will be developed that will enable various databases to be consolidated for their high-level use. By using the aforementioned various data, the various theories and empirical rules will be evaluated for their applicability, and attempts will also be made to discover new theories and empirical rules from the correlations between data.

(c) Explaining the manufacturing process of ceramics-based materials from a microscopic level and establishment of their process design technology

Properties of ceramics-based materials are in most cases dependent on their raw materials and their manufacturing process, and this is one of the causes contributing to the difficulty of their material design. By explaining the correlations between the phenomena and processes occurring in the process from raw material to finished goods and the resultant microstructures and organizations, guidelines will be established for the design of materials, to include the process. Also, by building various models, the simulation technology will be established that will enable the result to be forecast from the process control parameters. The work will be conducted systematically with the cooperation of the various experiment and observation groups, the theoretical research groups conducting research from microscopic levels using the methods as described in (a), and simulation groups, and the data and achievements thus obtained will be built into a database.

(d) Preparation and establishment of theories for forecasting properties of ceramics-based materials

Properties of ceramics-based materials such as strength, fracture, toughness, and various interface phenomena are important properties, but little is known of the mechanisms that trigger those properties and the factors that govern them. Among the causes for the lack of knowledge are problems specific to ceramics-based materials, such as the difficulty of obtaining specimens in which impurities are well controlled, and the fact that since the phenomena in the intermediate domain between the microscopic and the macroscopic domain often govern the properties of ceramics-based materials, the correlations between their microstructures and their macroscopic properties are not yet fully explained. If the qualities of ceramics-based materials are to be stabilized and if their material design technology is to be established, these problems must be solved. Therefore, experiment and observation groups will be organized for each of the phenomena, and, with the cooperation of theoretical research groups conducting research from microscopic levels using the methods described in (a) and macroscopic theoretical research groups, they will work systematically to clarify the problems and try to establish the theories for forecasting the material properties of ceramics-based materials.

(e) Building a comprehensive material design system for ceramics-based materials

A material design support system will be built by putting together the achievements of the research and development activities mentioned in paragraphs (a) through (d). The materials design and forecasting theories and methods, to include the processes, will be established at each of the R&D hierarchies and levels described in paragraphs (a) through (d) and the results will be consolidated into a system. Further, a system will be established by organically linking the databases and general-purpose software established in the core R&D activities described in paragraphs (a) through (d) with theories and methods.

For example, this system will inform a researcher engaged in the development of a material of the theories and empirical rules needed to forecast and design the material's properties and characteristics and will provide him with various input data. It will also present the researcher with the required manufacturing process conditions. Software will also permit the researcher to conduct simulations to forecast the material's characteristics. For a researcher intending to clarify some specific phenomenon of a material, the system will present to him various relevant theories so that he will be able to conduct theoretical calculations and simulations best suited to the concerned material systems.

(3) Structure for Research Promotion

Research associations will be organized according to the research projects described in paragraphs (a) through (d), with each association pursuing this research theme on a long-term basis. The group in charge of research theme (e) will coordinate the overall progress of the projects and will establish a comprehensive system based on the achievements obtained in (a) through (d). A central research organization equipped with a large number of supercomputers will be established, thereby ensuring enough computer resources for the research groups; it will also be responsible for the custody and operation of various databases, general-purpose software, and materials design support systems, as well as for their widespread use.

8. Supplement (Questionnaire)

8.1 Objective of the Questionnaire Survey

In order to advance promotion of fine ceramics R&D and its growth as an industry, the "Survey and Research on Materials Science of Fine Ceramics" Committee, under a contract from the Ministry of International Trade and Industry (MITI), is undertaking a survey and research on the current state of qualitative stabilities of fine ceramics and their future tasks and on the applicability of materials science-based approaches to fine ceramics. This is aimed at clarifying the future directions of the quality stabilizing technology and new materials development technology.

The objective of the current survey is to gather directly from people engaged in R&D of fine ceramics (including glass and cement) or its manufacture their opinions on the current problems of fine ceramics technology and its prospects and on the needs for materials science-based approaches to the technology. The findings will be reflected in the survey report.

8.2 Contents of Questionnaire

Q1: Mark with a circle your organization and your job.

- (1) a. Enterprise b. University c. Government research institute
 d. Other ()
- (2) a. Research and development b. R&D planning and management
 c. Manufacturing and production control d. Other ()

Q2: Enter the kinds of materials you mainly deal with and the targets of your research (in as much detail as possible). (Examples: Development of ceramic engines using silicon carbide; fracture characteristics of structural ceramics.)

Q3: From the perspective of promoting your own research or from that of developing or manufacturing excellent materials, or realizing qualitative stability, enter in as much detail as possible what problems you are facing today, what are the tasks that you must solve, and what phenomena you must explain. (Examples: A change in the lots of the raw material powder gives the manufactured electronic material-grade ceramics a large scatter in their properties; it is necessary to establish a high-precision evaluation method of raw material powder.)

Q4: If various problems and conditions associated with the development and manufacture of fine ceramics are to be solved or if improvements are to be found to those problems, and if materials featuring epoch-making technological advances are to be developed, we consider the applications of materials science-based approaches to fine ceramics (theoretical explanations of various phenomena, development of theories, empirical rules and various databases, and the design of materials and processes thereof). In this respect, give answers to the following questions:

(1) In connection with Q3, or generally speaking, what do you think of the slowness with which the work for theoretical explanations of fine ceramics (including glass and cement) is progressing? And what spheres and phenomena of fine ceramics do you think are laggards in terms of the development of theories, empirical rules, and databases? (Examples: Microscopic mechanisms of fracture, and so forth.)

(2) If you have any concrete requests with respect to fine ceramics, such as finding solutions to their problems and their phenomena, or establishing databases, theories, and empirical rules for them, enter them.

(3) Conversely, if you have any knowledge of the spheres and phenomena of fine ceramics where the work for their theoretical explanations and the establishment of their theories, empirical rules, and databases are relatively well advanced, enter those spheres and phenomena. If you are using any theories, empirical rules, or databases, enter them.

Q5: Thanks to recent advances in various theories and computation methods and to the rapid growth of computation means such as supercomputers, (a) theoretical calculations on the microscopic levels and the explanation of phenomena using simulations and the design of materials and (b) attempts at development of materials design systems that combine various databases, theories, and empirical rules have been conducted in various materials fields. In connection with the trends of trials as described above, answer the following questions (if possible, give separate answers to paragraphs (a) and (b)).

(1) If your research group has ever tried or succeeded in explaining the phenomena as described above or in materials development, or if your research group has ever tried or succeeded in the construction of materials design systems as mentioned above, write down the outlines of the trial or success briefly. Or, if you have any knowledge of such a trial or a success by any other research group, write it down.

(2) If you think there are some phenomena or fields where special efforts are being called for to explain the phenomena and to design materials, described above, write them down.

(3) In relation to the trials to explain the phenomena and for materials development, give your frank opinion on their prospects or potential, or what expectations or criticisms you have of them.

(4) Regarding the general use of computers in research and development, give in as much detail as you can the current state of computer utilization in your company or by your research group, your company's or your research group's plans or prospects for computer utilization in the future.

Q6: Regarding the direction of research as indicated by the underlined parts in Q4 and Q5, if you consider that they should be organized as national projects, or that they should be undertaken by universities and government research laboratories, enter your suggestion (examples: They should be organized as large-scale MITI projects; they should be built as joint databases; and so forth).

Q7: In the research and development of materials in general, if you have any knowledge of a case in which any unique idea or insight, a discovery or a change has led to an advance in research and development, enter it. Regarding the research environment or the research system that nurtures such unique ideas or insights, if you have any proposals of requests, enter them.

8.3 Summaries of the Questionnaire Survey Results

Q1: Respondents' affiliations

Table 1 shows the results of Q1-(1).

Table 8.1 Results of Q1-(1)

Enterprises	Universities	Government labs	Others	Total
90	157	42	0	289

Table 8.1.2 shows the results of Q1-(2).

Table 8.1.2 Results of Q1-(2)

	Enterprises	Universities	Government labs	Others	Total
Research and development	70	113	39	0	222
Planning and management	10	1	3	0	14
Manufacturing	6	0	0	0	6
Others	5	43	1	0	49

Q2: Research targets

The survey results were classified into "materials" and "research targets." Materials were further subdivided into structural materials, functional materials, traditional materials (glass, cement, etc.), and others. Research targets were subdivided into process research, evaluation research, and parts and devices development research. The results are shown in Tables 8.2.1 and 8.2.2.

Table 8.2.1 Results of Q2 (classified by material type)

	Enter- prises	Univer- sities	Govern- ment labs	Total
Structural materials	41	40	11	92
Functional materials	34	41	19	94
Traditional materials	8	8	3	19
Others	8	39	9	56
Total	91	128	42	261

Table 8.2.2 Results of Q2 (classified by research target)

	Enter- prises	Univer- sities	Govern- ment labs	Total
Process	23	58	14	95
Evaluation	12	35	4	51
Parts development	24	9	5	38
Total	59	102	23	184

Q3: Problems and tasks

The following opinions were raised.

(1) Standardization is incomplete

- Different measuring methods generate different data
- Manufacturing conditions are not described in the catalogs

(2) "Materials" are in short supply

- High-purity raw materials are not available
- Equipment is not available
- Research money and manpower are in short supply

(3) Data are not available

- Relations between additives and material properties
- Phase boundary energies, thermal properties, etc.

(4) Theories are not available

- Principles common to amorphous and crystalline materials
- Forecast of the amorphous domain
- Clarification of the control factors in processing
- I want to produce a new multicomponent glass without conducting any experiment and forecast its properties
- Bonding mechanisms

(5) Methods are not yet established

- Methods to evaluate fracture toughness in composites
- Methods to evaluate strength of fibers
- Nondestructive testing methods
- Processing methods and strengths

(6) There are problems with scattering

- Fluctuations in the raw material lots
- Reproducibility of material property values in products

(7) The efficiency is not high

- Processing
- Long time and high temperature are needed for sintering

(8) The costs are high

- Analysis equipment
- Processing cost
- Raw materials

Q4-(1): Areas and phenomena where research and development is lagging

	Private sector	Univer- sity	Total
1. Mechanisms of fracture phenomena and fatigue	12	17	29
2. Theories and mechanisms of sintering	7	16	23
3. Interface/phase boundaries	14	13	27
4. High-temperature properties (thermo-dynamic considerations)	0	8	8
5. Databases addressing mechanical properties such as K_{IC}	0	7	7
6. Compaction theories	0	8	8
7. Thin films/properties evaluation methods	0	1	1
/interface structures	0	1	1
/growth processes	2	1	3
8. Glass and water solutions			
Thermodynamic	0	2	2
Crystallization mechanisms	0	6	6
Local structures of atoms	1	8	9
Others	1	7	8
9. Piezoelectric databases	0	1	1
10. Design methods of microscopic structures and ceramics	2	2	4
11. Atomic and molecular approaches (to include fracture)	0	10	10
12. Rheological natures (deformation, flow)	0	1	1
13. Mechanical processing mechanisms (including damage)	2	3	5
Their evaluation methods	0	2	2
14. Concrete and repair	0	1	1
Alkaline reaction mechanisms	2	1	3
Hydration reactions of cement	3	2	5
15. Databases for biomaterials	0	3	3
16. Optical effects	0	1	1
17. Superconductivity and mechanisms	2	4	6
Characteristic data	0	1	1
18. Semiconductor mechanisms	0	1	1
19. Databases for dielectrics	1	1	2
20. Methods of forecasting impurity effects and selection of additives	0	5	5
21. Analysis of trace amounts of inclusions	2	1	3
22. Elucidation of diffusion phenomena (to include those under high temperatures)	1	4	5
23. Crystal plasticity mechanisms	0	2	2
24. Ceramics/metals interaction	2	2	4
25. Databases for crystal structures of ceramics	0	2	2
26. Corrosion science field	3	3	6
27. GFM design	0	1	1

[continued]

	Private sector	Univer- sity	Total
28. Databases for manufacture of raw material powders	6	5	11
29. Standardization of raw material elements (including their properties)	0	4	4
30. Processes and properties (including volume-production technology)	2	7	9
31. Making public the manufacturing methods	6	14	20
32. Manufacturing methods of madreporic bodies with micropores	0	1	1
33. Making public the manufacturing methods	1	2	3
34. Mechanisms of how to produce composites	0	4	4
35. Phase diagrams (including grains)	2	2	4
36. Relationship between functionalities and properties and crystal structures	2	1	3
37. Mechanisms of self-repairing materials	3	1	4
38. Theories of color tones and transparency	3	1	4
39. Materials science general Research being done by people ignorant of the science's true nature The science is empirical Research is being done with no coordination between researchers	4	13	17
40. No reply	No count	8	
41. Catalytic materials	1	0	1
42. Sol-gel process	3	0	3
43. linkage with physics	1	0	1
44. Tribology	2	0	2
45. Heat conductivity databases	1	0	1
46. Properties of porous bodies	1	0	1
47. Powder engineering	6	0	6
48. Reliability	3	0	3
49. Thermal stress	3	0	3
50. Material strength	10	0	10
51. Mechanisms of conductivity	1	0	1
52. Physical properties	4	0	4
53. Composite databases	1	0	1
54. Reaction mechanisms	1	0	1
55. Compositions vs. properties (theories, databases)	4	0	4
56. Materials design	2	0	2
57. Control of microstructures	1	0	1
58. Creep characteristics	3	0	3
59. Temperature measuring technology	1	0	1
60. Cement: microstructure/composition	3	0	3
61. Materials evaluation methods	2	0	2
62. Rheology	2	0	2
63. Defects	1	0	1
64. Thermodynamics databases	1	0	1

Q4-(2): Areas and phenomena where research and development is lagging

	Private sector	Univer- sity	Total
1. "I will do it by myself"	0	3	3
2. Sintering theories (to include reaction mechanisms)	1	5	6
3. Compact structures and density control	0	2	2
4. Interactions between dispersants	0	1	1
5. Composite theories (micros to nanos)	0	2	2
6. Manufacture of single crystals (SN)	0	1	1
7. Process of thin-film growth	0	1	1
8. Correlation between process parameters and composite material properties	5	5	10
9. Properties of microstructures	0	4	4
10. Improving K_{Ic}	0	1	1
11. Evaluation methods of properties (under high temperatures)	0	2	2
12. Grain boundary structures and electric characteristics	0	1	1
13. Evaluation methods of defects on machined surfaces	0	1	1
14. Interface phenomena (bonding, fracture)	3	5	8
15. Mechanisms of fatigue	1	1	2
16. Main factors of synthesis processing methods, their scope of application	0	1	1
17. Clarification of state of atoms in ceramics solids	1	2	3
18. Clarification of phenomena of non-equilibrium, nonuniform reaction systems	2	2	4
19. Concentrated suspensions			
Measurement and theory of jitter voltages	0	1	1
Dispersant conformations	0	1	1
20. Mechanisms of high-temperature superconduction	1	1	2
21. Conditions for adjustment of perovskite oxide compounds	0	2	2
22. Defect structures of grain boundaries in oxides	0	1	1
23. Mechanisms of crack generation in heterogeneous bodies of concrete, etc.	0	1	1
24. Explanation of intermediate structures in glass	0	1	1
25. Characteristics of structures of glass of high ionic conductivity	0	4	4

[continued]

	Private sector	Univer- sity	Total
26. Mechanisms of crystallization	1	1	2
27. Thermodynamic approaches	0	1	1
28. Basic experimental methods (including examples of failures)	0	1	1
29. Various properties and theories	2	2	4
30. Relationship between mechanical process- ing mechanisms and levels of difficulty	0	1	1
31. Mechanisms of conduction in solid substances	0	1	1
32. Dispersion in composite materials and their properties	1	0	1
33. Fine ceramics general	1	0	1
34. Fracture simulations	1	0	1
35. Powder engineering	2	0	2
36. Color and light vs. material	1	0	1
37. Glass phase splitting	1	0	1
38. Sol-gel process	1	0	1
39. Mechanisms of genesis of functions	1	0	1
40. Synthesis and reaction mechanisms	2	0	2
41. Dielectric theory	1	0	1
42. Fracture mechanisms	3	0	3
43. Mechanisms of organization of structures	1	0	1
44. Creep characteristics	2	0	2
45. Grain boundary strength	1	0	1
46. Abrasion and friction	1	0	1
47. Corrosion resistance	1	0	1
48. Reliability and durability	1	0	1
49. Cements (reaction, properties, rheology)	1	0	1
50. Tribology	1	0	1
51. Catalysts	1	0	1
52. Grain diameter/surface phenomenon	1	0	1
53. Systems that foster ideas	1	0	1

Q4-(2) Desired databases

	Private sector	Univer- sity	Total
1. Thermodynamic data (including under high temperatures)	4	3	7
2. Phase diagrams of multicomponent systems	2	4	6
3. Diffusion data (including those for solids)	1	5	6
4. Interfaces			
1) Surface energy	0	1	1
2) Interface vs. property value	1	1	2
3) Nonoxide metal synthesis	0	1	1
5. PAT (ceramics)	0	1	1
6. Sintering	2	3	5
7. Accurate characteristics of raw materials	2	3	5
8. Property values			
1) Mechanical characteristics at high and low temperatures	0	12	12
2) Reliability of ceramics	0	1	1
3) Composites and properties	0	2	2
4) Shape dependency	0	1	1
5) Machined surface vs. strength	0	2	2
6) Electrical characteristics	0	1	1
9. Intermediate distance structures (glass) vs. properties	0	1	1
10. State of applications in structural bodies	0	1	1
11. Crystal structures (to include single crystals)	2	6	8

Q4-(3) Theories

	Private sector
• Compositions of glass and their macroscopic properties	2
• Materials design of glass/expert systems	2
• An expert system for sintering and strength of Si_3N_4	2
• Vibration propagation theory (macrocracks, crack diameter and crack volume forecasting)	2
• Vitrification domain	1
• Material strength theory (linear fracture dynamics)	1
• Empirical rules for actual products	1
• Material design for superalloys (In-base superalloy)	1
• Molecular design for medical drugs	1
• Metallurgy reaction engineering	1
• Simulations for forecasting properties of dielectrics	1
• Simulations of growth process of ceramics	1
• Forecasting heat stress characteristics in piezoelectric products ("aurenius" filing model)	1
• Voltage multiplied by the third power rule and temperature 10°C rule in dielectrics	1
• Weibull statistical analysis	2
• Fracture mechanics	2
• Microstructures and characteristics of ceramics	1
• Thin-film growth simulation	1
• Piezoelectric sensors (Putley type)	1
• Behavior of hydroxyl groups on surface of metal oxides	1
• Analysis of functional groups and adsorbing species on surface of grains	1
• Sintering theory	1
• Rheology	1
• Hertz crack theory	1
• Glass domain and properties	1
• Shape design of ceramic parts by FEM	1
• Theory of colloid chemistry	1
• Additive rule (glass)	1
• Light-emitting characteristics (rare earth elements)	1
• Darcy's law	1
• Carman/Kozeny equation	1
• Empirical rules for the design of glass materials	1
• Sintering/strength expert systems	1
• Mechanical characteristics testing in metallic materials	1

Q4-(3) Databases

	Private sector
• X-ray diffraction databases	4
• Phase diagrams and state diagrams	3
• PATOLIS	2
• JOIS	1
• Thermodynamic databases	4
• Liquid phase synthesis databases (alkoxides)	1
• JICST (Japan Information Center for Science and Technology)	3
• Corrosion resistance data "Handbook on Corrosion Resistance of Ceramics"	1
• Databases for ceramic parts	1
• Magnetic materials	1
• Glass databases	3
• Lambert-Bernstein	2
• Databases for analysis and spectroscopy of elements	1
• Databases for metals	1
• Databases for heat conduction	1
• Databases for silicon single crystals	1
• Databases for zeta potential and relative surface area in particles	1
• Databases for friction coefficients	1
• Databases for methods of metals-ceramics bonding	1
• TEM databases for metal-ceramic interfaces	1

Q5-(1) and Q5-(2)

With respect to theoretical calculations, simulations, and materials design systems, answers to the questions Q5-1: actual cases and Q5-2: phenomena and areas that need to be clarified in the future are tabulated below. These answers contain only those that are considered substantial in content, and include a few macroscopic (bulk samples) simulations.

	Private enterprises	Universities and colleges	National and public laboratories	Total
Number of questionnaires recovered	85	134	41	260
Number of answers to Q5-(1)	33 (39%)	44 (33%)	11 (27%)	88 (34%)
Number of answers to Q5-(2)	61 (72%)	72 (54%)	17 (41%)	150 (58%)

One in three respondents replied that they knew of cases of trials or successes in the attempts at items described in Q5-(1) and Q5-(2), and most of them were related to research by research groups in the Japanese universities and government laboratories. Private enterprises were found to have strong, concrete needs in connection with the item on the questionnaire, "phenomena and fields that must be clarified in the future."

Q5-(1) can be summed up as follows:

(1) Theoretical calculations and simulations

For structures, the bulk of simulations still consist of those at macroscopic levels (bulk samples). However, an approach based on the solid electron theory is being tried in part. For functions, theoretical calculations are mostly being done on electrical properties such as the dielectric constant and the mechanism of conduction. Regarding processes, as with structures, macro-level simulations are being mainly tried. For glass, many examples of molecular dynamics computation of their structures and the transport phenomena were presented. Some respondents replied, "Although our groups are not committed now, we want to undertake research projects in the future."

(2) Empirical rules and systems

Some cases were reported in which thermal thermodynamic databases and the materials design work for ceramics and glass have been replaced by expert systems. Such instances are still few compared to similar cases for theoretical calculations and simulations.

Q5-(1): Theoretical calculations and simulations (actual cases)

Structures:

- Structure and stability of interface in ceramics
- Relations between microstructures and toughness and strength
- Crack pattern, and the process of dislocation and emission from cracks
- Numerical fracture mechanics

Functions:

- Mechanism of conduction in varistors
- PTC simulation and BaTiO_3
- Dielectric and piezoelectric characteristics in $\text{Pb}(\text{Zn}, \text{Nb})\text{O}_3$ - PbTiO_3 systems
- Simulation of electric conductivity in SiC sintered bodies
- Calculation of electronic structures of Al_2O_3 and SiC
- Calculation on the band in semiconductors and superconductors
- Forecast of the properties of electronic materials
- Simulation of characteristics in magnetic core materials
- Simulation of super-ion conductors
- Material design of "Nacicon" ($\text{Na}_3\text{Zr}_2\text{Si}_2\text{PO}_{12}$)

Processes:

- Simulation of the process of adhesion of grains in slip casting
- Simulation of forming, sintering, and solidification
- Simulation of chemical vapor deposition (CVD)

Phase changes in glass:

- Crystal structure, forecast of the stabilized phase
- Structure, composition properties (to include optical functions) and crystallization in glass
- Transport phenomenon in glass and molten salts
- Dispersion and reaction of organic particles in zeolite pores
- Phase diagrams, dielectric constants and lattice constants for solid solutions
- "Spinodal" dissolution of $\text{SnO}_2\text{-TiO}_2$ and others
- Explaining the cause for the high elasticity of "oxynightlight" glass

Others:

- Thermal stress and residual stress simulation by device simulation

Q5-(1): Empirical rules and systems (actual cases)

- Thermodynamic equilibriums and phase diagrams for multicomponent systems
- Construction of a thermodynamic database and its application to electrodes for solid fuel cells
- An expert system for selecting sintering additives for silicon nitride and silicon carbide
- An expert system for forecasting generation of perovskite
- A glass expert system (forecasting thermal expansion and the Young's modulus)
- A ferrite design system
- A support system for helping the design of raw materials for NTC thermistors
- Forecasting the corrosion resistance of metals and alloys from their thermodynamic characteristics

- Estimating the heating volume reduction curve for compounds for injection molding
- Estimating the theoretical strength of ceramics from their thermal expansion coefficient
- Design of SiC/C gradient functional materials

Q5-(2): Phenomena and areas requiring explanations in the future

Structures:

- Forecast and design of mechanical characteristics—analysis of fracture and fatigue mechanisms in ceramics, life estimate, higher toughness
- Behavior under special environments and critical conditions: high temperature, different atmospheres, rigorous thermal and dynamic conditions, space environment
- Materials design of nanocomposites (forecasting characteristics at nano levels)
- Interface and surface problems: characteristics of grain boundary phases and control of the grain boundaries; stress mitigation, fracture of bonding surfaces, and surface energy; gradient materials; and microstructures of surfaces

Functions:

- Optically functional materials (photorecording materials)
- Theoretical calculations of function-generating mechanisms in electronic ceramics
- Mechanism of electric conduction (varistor, thermistor, superconducting materials)
- Dielectrics high Q and high ϵ (microwave dielectrics), low Q_m (piezoelectrics)
- Mechanism of ionic conduction, and ion expansion
- Generation of defects by optical excitation
- Mechanism of gas sensing

Processes:

- Reactions (nitric reaction, and so forth), catalytic reactions
- Sintering process
- Powder processing
- Alterations in properties by processing
- Clarification of friction and abrasion
- Preparation of powders by sol-gel method, thin-film synthesis process
- Thin-film phenomenon
- Flame injection phenomenon
- Precision processing

Phase changes in glass:

- Crystal structure, glass (amorphous) structure and properties
- Transparency-loss phenomenon in glass
- Precipitation process of ultrafine particles
- Coagulation process of particles
- Mechanism of crystal growth (including the generation of nuclei)

Materials:

- Structure, electron, functions, bio-, optical, artificial super-lattice, semiconductor, amorphous materials, fiber, superconductor, superhigh temperature materials, porous bodies, solid fuel cells, plastic materials, pigments, PTC thermistor, gradient functional materials, compound materials, fiber-reinforced metals/fiber-reinforced ceramics, particle-dispersed reinforced materials, precursor ceramics

Others:

- Databases for various characteristics of ceramics
- Deciding the interatomic potential for simulation
- Nondestructive testing technology

Q5-(3): Trials at explaining phenomena and at materials development; their prospects and possibilities

(Number of answers)

	Univer- sities and colleges	National and public labora- tories	Private enter- prises	Total
Number of questionnaire forms recovered	141	37	82	260
Number of answers	79 (56%)	19 (51%)	58 (71%)	156 (60%)

(Outlines of answers)

(Universities and colleges)

Forty-seven of the 79 respondents expressed expectations, either positively or conditionally. Eighteen gave passive or negative opinions, and 14 gave other opinions.

Some of the expectations: "I believe these trials will ultimately succeed. Since existing models are too simple, they may not find much use in practical applications, but the projects must be undertaken from a long-term perspective of 10 to 20 years," "These research projects will contribute greatly to materials development in the promising fields such as nonlinear optics," "Where it is difficult to glean facts from experiments, such as in MD, simulations are highly effective. They can point out problems that experiments failed to disclose," "It is necessary to start research with an eye to 10 years from now."

There were many opinions emphasizing the need for interchange between experiment and theory. Some examples: "Experiment and theory must maintain a relationship as if they are the two wheels of a bicycle. If a researcher is going to construct a theory of his own, he will have to have exchanges with researchers in fields other than his own, by forming a research group or groups," "Comparing the data obtained in a simulation with the actually measured data will raise the accuracy of the simulation and produce results of high practical value."

Even among those who expressed high expectations, many pointed out problems with simulation and materials design. Some examples: "MD still is not powerful enough to explain problems associated with, among others, electrons. On the other hand, in molecular orbit computation, the numbers of atoms that can be factored in are too small, and this makes it impossible to obtain group information. Problems like this must be solved," "Since ceramics are complex

systems, the desired form of computation is something that shows there are limits to calculations or that gives guidelines, and I don't think the kind of calculation methods that take in facts as they are will achieve any appreciable results," "Since macroscopic behavior is affected by many phenomena, it is very difficult to discuss behavior from microscopic-level results. The research task for the future is to find out what can bridge the two."

A large number of opinions pointed out the lack of theories and empirical rules for ceramics. Examples: "Rather than expending our energy, trying to make our findings conform with imported theories like fracture mechanics, we should make steady efforts to explain the intrinsic nature of ceramics and establish the findings as the laws of science," "The most important thing is to have an accumulation of results of measurements and to establish empirical rules."

Among the negative opinions, views that "such trials will not lead to discovery of new phenomena" were most numerous. Some examples: "For the optimization of compositions and processes, the application of materials design systems is most important, but such systems will not lead to new discoveries or new findings," "The proposed materials designs as they are now are hardly sophisticated enough to create new materials. Some systems that make it possible to create new materials are needed," "I think such trials at explaining phenomena and at development of materials will gain further importance in the future, but correlations between theories and actual materials should always be kept in mind."

On the other hand, a large number of the respondents cited the need to build databases. Examples: "I think Japan has no organization charged with the collection of basic data on thermodynamic values, state diagrams, X-ray analyses, and so forth," "Rather than relying on calculations alone, we should make efforts to accumulate accurate data and collect data for databases. Researchers who produce data deserve much more respect," "The most important thing is to keep on compiling databases."

(National and public laboratories)

Thirteen of the 19 respondents expressed positive or conditionally positive expectations. Four gave passive or negative opinions, and two were ambivalent.

Even among those respondents who expressed high expectations many pointed out problems and tasks. Some examples: "Modeling of a complex phenomenon is possible by breaking it into simple pieces and by exploring those pieces theoretically and this in turn will enable one to design a new material with excellent properties as were forecast theoretically. However, an excessive reliance on theory may lead one to skimp on experiments and thereby to overlook complex data obtainable only with actual measurements, and this, I fear, may make his work out of touch with reality," "I think they are important, but most of the discussions are being waged on the assumption of ceramics at their idealistic state, which is far away from what ceramics are in reality. The problem is how to narrow down the gap between the two."

There were many opinions emphasizing the need for increased exchanges between research groups or with research groups in other fields of science: "If a close linkage is maintained with other experimental groups and groups of materials engineers, a big advance can be expected," "My hope is to establish a method of simulation, and to that effect, it will be necessary to understand the phenomenon by conducting experiments systematically," "Cooperation must be maintained among researchers in solid physics, metals, and ceramics. Considering that most of the ceramics makers have their roots in chemistry and that their ideas are firmly entrenched in the messy field of manufacturing, there are limits to how far they can make headway. A forum is needed where researchers of different disciplines can get together. An academic society highly geared to topics like MRS is promising."

(Enterprises)

Forty-two of the 58 respondents expressed positive or conditionally positive expectations. Ten gave passive or negative opinions. Six were ambivalent.

These opinions were of the same patterns as those expressed by the universities and colleges, and some of them are described below: "The previous method of going after any material that you can lay your hand on under the mentality, 'first, there is a development and an evaluation will follow it,' won't fly any more. It is necessary to conduct materials design based on theories and databases," "These trials are absolutely necessary for the development of higher-performance ceramics, and the government should take leadership in executing those projects," "For the development of high-quality materials and new materials, such scientific approaches will become indispensable," "With the progress of computer technology, the tendencies will become more apparent. A social system is desired to be in place where the protection of software and its widespread use can coexist."

There were also many opinions calling for the collaboration between experiment and theory. Some examples: "I am expecting that the experimental approach using TEM and AE and the computer simulation based on theory will work side by side to gain correct understanding of fracture of ceramics," "A cooperative system must be in place where the results of calculation methods based on physics-like ideas can be confirmed by chemistry-like experiments."

Among the problems and tasks for now: "Cases are found in which there exist gaps between analyses such as theoretical calculations and simulations and actual data, and it is about time analyses be conducted to narrow these gaps," "In ceramics there are still big gaps between their calculated values and their actual values. In ceramics, in some cases, the surface and grain boundaries are more critical than the bulk, and the state of excitation and the lattice vibration also play a part. As the technology stands now, it is impossible to explain such phenomena up front, but the establishment of some calculation methods that enable those phenomena to be explained is awaited," "In structural ceramics phenomena occur on macro-levels, so existing calculation techniques are unable to predict them," "Structural ceramics are greatly affected by their manufacturing processes. As the technology stands now, in structural ceramics there is a great obstacle to be surmounted if

theoretical calculations are to be translated directly into superior products."

Among other opinions calling attention to the lack of theories and empirical rules: "The most important thing is how to theoretically explain the phenomenon of materials whose phenomenon has yet to be explained. University people on whom great hopes are placed to come up with theories are content themselves with merely making announcements, 'we have succeeded in trial manufacture of such and such materials,'" "Many of the ceramics theories are borrowed from the science of metals, and the science of ceramics has much room for growth in the future. I don't think preparing databases in haste will do any good in producing the expected results."

Among the negative opinions: "The trials to explain phenomena are considered highly promising, but the attempts at materials development will be very difficult," "A new breakthrough comes from a unique idea, so I don't have much trust in the talk that computers will create new materials."

There were many opinions emphasizing the need for the accumulation of basic data and the construction of databases. Some examples: "I believe theoretical analyses by computer and computer simulations will prove to be effective means for developing the designs of materials and their manufacturing technologies in the future, but the levels of accumulation of required basic data are unsatisfactory," "I am expecting that in the future, materials development will proceed from theoretical considerations in the field of ceramics as well. In this context, the number of databases must be substantially increased," "Related companies are asked to come forward with data in their possession to put for the guidelines."

Q5-(4): Use of computers in research and development

(Number of answers)

	Univer- sities and colleges	National and public labora- tories	Private enter- prises	Total
Number of questionnaire forms recovered	141	37	82	260
Number of answers	74 (52%)	16 (43%)	57 (70%)	147 (57%)

(Outlines of answers)

(Universities and colleges) and (national and public laboratories)

Almost all respondents replied that they have either been using or plan to use computers in the future. However, the number of people who replied, "We have been using mainframe computers or supercomputers," accounted for only about 10 percent of the respondents, and the rest were using computers at the laboratory levels, i.e., personal computers. Personal computers are used for such applications as the control of various experimental equipment and automated measuring, analysis of crystal structures, two-dimensional image processing, processing and analysis of various data, word processing. Among large-size calculations are thermal stress analyses by the finite element methods, simulations of cracks on boundary surfaces, multicomponent equilibrium calculations, electric conduction simulations, combustion gas flow simulations. Some of the opinions: "I would like to have a high-speed computer with a capacity to conduct molecular orbit calculations and simulations," "I plan to prepare a knowledge database containing molecular calculations as well."

Some university people pointed out the high cost of rentals of large-size computers. It seems that large-scale calculations have until now been conducted in those fields of calculation where software is available, such as the finite element method. The reasons why the use of computers for conducting theoretical calculations on the macro-levels and simulations is limited to a small number of specialists seem to be the high cost of computer rental and the lack of software.

(Enterprises)

Almost all of the respondents have either been using or plan to use computers. In companies as well, such operations as the control of experimental equipment, data processing, and image processing and analysis are being conducted, as with the universities, using personal computers and others. But as can be seen from the answers "the solvers for structural analysis, heat conductivity analysis, and fluid analysis are incorporated in the mainframe and access to it can be had via workstations," and "computer use mainly consists of computer chemistry centered on molecular design and engineering support centered on structural analysis," computers are also being used to conduct large-size calculations mainly in those areas where software is in circulation, such as the stress analysis, structural design, heat conduction and flow, device simulation, and molecular calculation fields. However, as can be seen from the opinion, "Large-size calculations using computers are becoming indispensable in product design, reliability evaluation, circuitry and device simulation, but when it comes to materials development, there is no software of any utility. Therefore, the priority is how to train talented people who have good knowledge of materials science and simultaneously are endowed with mathematical abilities," in the companies surveyed as well, the use of computers in explaining phenomena on the macroscopic levels and in materials design seems to be not progressing smoothly because of the software and personnel bottlenecks.

However, as for the future directions of computer use, many positive opinions have been received. Examples: "By focusing our research to several ceramics for use as electronic materials, we plan to construct materials design support systems for them. We also plan to conduct experiments using models to raise simulation accuracy as well as actual experiments for verification," "Computers are routinely employed in the molecular design of organic polymers, and this should be the case with ceramics," "The actual state of computer utilization is that computers are being used in the calculations of databases and relational expressions for experimental data. They should be used from now for verifying the mechanisms of fracture and for designing materials based on the findings," "We hope to explain reactions by means of quantum science calculations." Movements are seen on the part of individual companies to produce their indigenous databases, as can be seen from the following observations, "It seems our company is going to compile a company-wide database," "We are going to develop a research and development database."

Q6: In connection with the promotion of research and development in the lines of direction as described in the underlined parts of the texts in questions 4 and 5, what do you expect of, in concrete terms, the national projects, universities and national and public laboratories?

(Number of answers)

	Univer- sities and colleges	National and public labora- tories	Private enter- prises	Total
Number of questionnaire forms recovered	141	37	82	260
Number of answers	59 (42%)	9 (24%)	46 (56%)	114 (44%)

(Outlines of answers)

(Universities and colleges)

Forty-seven of the 57 respondents replied that some kinds of research projects, such as "large-scale projects on the materials design for glass and ceramics by the Ministry of International Trade and Industry" and "execution of research projects under the Ministry of Education, Science and Culture's research priority program," are needed. As for the contents of the requested projects and the issue of how they should be executed, the following opinions were raised: "Basic research-oriented projects," "Computational physics projects where achievements in terms of commercial applications are not being strongly sought," "In organizing research groups, autonomy of the individual research organizations should be honored to the highest degree," "The walls

separating the Ministry of International Trade and Industry, the Ministry of Education Science and Culture, and the Science and Technology Agency from one another should be brought down," "Only a few select companies are being allowed to participate in the projects at present," "Projects should be managed in a manner that allows the participation by private universities."

Many opinions were received that called for the government to undertake the job of compiling databases: "Databases which all researchers can access are needed (databases for crystal structures, thermodynamics, etc.)," "Databases that contain information on experiment methods and evaluation methods as well should be constructed in collaborative projects involving government, industry, and academia," "By instituting a structure of cooperation under which some people devote themselves to the gathering of data while others compile those data into a database, it is hoped to build up a system over a period of 10 years or so," "An organization that undertakes accumulation of basic data must be established."

On the other hand, there were many opinions calling for intensified efforts in basic research and creative research: "It is hoped that funds will be appropriated for unglamorous projects like basic research in inorganic materials science and the discovery of new functions. It may be easy to organize research projects in areas where the potential for development is high, but hopefully there will be room in research that permits a researcher to pursue his dreams, away from constructions for practical results," "There is no doubt about the importance of large-scale projects, but unless the eye is turned to what can be done to promote and develop individual unique research, nothing creative will come out of the effort," "Large increases in the funds for basic research, improvement of treatment of researchers, and improvement of the research environment," "The universities and national and public laboratories are in a desperate condition in terms of both personnel and funds."

(National and public laboratories)

Regarding projects, the following opinions were received: "The Science and Technology Agency will be able to mobilize the talents of researchers from different fields in the government and public laboratories, universities, and private enterprises by taking advantage of its project called the interdisciplinary basic research," "Large-scale projects are best confined in basic and theoretical fields. Where a concrete goal is set, the private sector will become secretive. Since compiling databases is a routine type of work, the operation is best left with private organizations like the Japan Fine Ceramics Association," "The database compilation project should have some built-in mechanism that guarantees continued generation of data into the future."

(Enterprises)

Forty-one of the 46 respondents gave opinions calling for the implementation of some national projects, such as "Since basic theories, calculation methods, and programs development are beyond the capabilities of individual research organizations of enterprises, these operations must be undertaken under a program of national project." Regarding the contents of these projects and the

issue of how they should be implemented, "After taking note of the problems that enterprises are finding very difficult to solve on their own, it is hoped that the Ministry of International Trade and Industry will implement large-scale projects as collaborative projects of government, industry, and academia will cooperate in the construction of large-scale databases for each of the fields. A center for training researchers in the aforementioned research must be built," "It is necessary to build a simulation program with some general-purpose capabilities and establish an environment where there is ready access to the program," "Since the number of researchers engaged in research on materials design of structural ceramics, their fracture dynamics and their reliability simulation is small, it is indispensable that researchers from other fields take part in the ceramics field," "It is hoped that a research organization will be established where the criteria for selecting its members will be more liberal and global, not necessarily based on the merit system such as social scale or record of achievements."

There were also many opinions calling for the construction of databases: "It is hoped that various databases will be built as national projects in accordance with some guidelines and guidance so that such things as complexity and wastefulness will be eliminated," "A firm commitment to contribute to the world and a firm financial backing are needed when embarking on the task of producing a database."

On the other hand, many opinions were raised by the enterprises calling for increased efforts for basic research by universities and national and public laboratories: "Universities and national and public laboratories should place more emphasis on basic research," "Enterprises expect the universities to undertake much more basic research. We expect them to explain the mechanisms of phenomena, to analyze structures and to build new theories," "It is hoped that the national and public laboratories will pursue a common theme and share the burden to see further progression of theoretical work."

Q7-(1): Examples where unique ideas or flashes, discoveries, or chance happenings have led to the progress of research and development in the research and development of materials

Universities and colleges

(70/115)

- (1) • Oxidation sintering in which metal powder and ceramic powder are mixed for developing a permeable type of ceramics
 - Powder extrusion forming using a water binder
 - High-performance grinding using a metal bond grindstone
 - Diamond grinding by the electrolytic dressing method
- (2) Centrifugal thermite process—The great precondition is that there are needs for the material.
- (3) It has been proposed that the surface energy is proportional to changes in enthalpy at both phases $\Delta H_f = T\Delta S_f$ (TL: liquid phase temperature, ΔS_f : melting entropy). A phenomenon on a microscopic scale is always in correspondence to a phenomenon on a macroscopic scale.
- (4) • Vitrified carbon
 - High-performance carbon fiber
 - C/C composite
 - SiC whisker (some cannot be listed because of trade secrets)

See CERAMICS, Vol 23, 1988, pp 1034-7 and CARBON, Vol 138, 1989, pp 162-6.
- (5) Professor Roy, Professor G. Petzow, Professor Jack
- (6) Intercalation of organic compounds into layers of layered crystals by reactions between solids
- (7) Development of new functional materials by means of dry mixing of water in the form of dry powder and ceramic powder
- (8) A composite of MO-Ti eutectic crystals, developed to make up for the defects of TiC, an element brittle under normal temperature, and MO, an element of low high-temperature strength, proved to have a lamellar structure and a high-temperature strength larger than that for pure TiC. A search for the cause revealed that TiC is solid solution hardened, and a probe for the latter cause revealed that solid solutions of TiC-ZrC have an exceedingly high resistance to high temperatures.
- (9) • PTCR: development of a varistor
 - Solid-phase epitaxy

[continued]

(10) Development of PZT, PTC: Routine but persistent research led to the development of the two (no special projects were organized). I have no knowledge of a case in which special projects have borne fruit in the form of development of commercial products.

(11) Intermediate layers for bonding are designed as having more than two layers, and the second layer is made of a metal layer with a lower thermal expansion coefficient (conventionally, a process was used in which the thermal expansion coefficient is made to change gradually, but in the new technique, the process is reversed). Bonding of turbos is an extension of the technology.

(12) While conducting an experiment on the claim treatment for tungsten contacts, the phenomenon of reaction between In-P alloy and W was observed. This finding led to the activated sintering of W and other applications.

(13) Hydroxyapatite containing water was turned into a form of ceramic. All conventional ceramics were anhydrides. The technique has contributed greatly to advances in bioceramics. It is best not to be a prisoner of fixed concepts of conventional wisdom.

(14) The cause of the fluctuations in the strength of a superalloy (WC-Co) and the range of strength the alloy is believed capable of attaining were estimated (1974).

(15) • Manufacturing method of flow sheet glass

• Research and development of ferrites

• Transition of stress-triggering phase in zirconia

• Discovery of ceramic sensor functions

(16) • Hitachi, Ltd.—SiC containing BeO (high-temperature conductive ceramic)

• British Honeywell Lab OR, U.S. ORNL (manufacture of grains of uniform grain diameter by sol gel method)

• Same as above (SiC by chemical vapor deposition (CVD), pyrolysis carbon coated fuel particles)

• Keihiko Yamada—Glassy carbon

(17) • Growth of molten liquid cooling method

• While conducting an experiment on the composition of an oxide superconductor, a student stayed at the bottom of the crucible [as published]

• The fused solid was treated, and the tester's needle swung much wider than is expected for metals

• It was found that superconducting phases precipitated during the cooling process

[continued]

(18) Development of conductive solid electrolyte using adamantine organic compound of nitride.

(19) Development of oxide superconductor—By forming a gel of alginic acid in an aqueous solution of Y, Ba, and Cu, the precursor is spun and sintered.

(20) Development of varistor, development of lucalox—The development of the crystallized glass owes to an accidental crystallization of glass as a result of a mistake in the experiment.

(21) Augite and feldspar of SiC and Al₂O₃ have been synthesized in aqueous solutions of normal temperatures. The clue to the success came from the fact that minerals such as augite and feldspar, which were believed to be authigenic [as published] are often found in natural sedimentary rock. (Patents have probably been obtained by Toshiba Corp.).

National and public laboratories

(16/28)

(1) Carbon fiber (Government Industrial Development Laboratory, Osaka).

(2) Development of Nd-B-Fe permanent magnet, APPLIED PHYSICS, Vol 56 No. 5. "I suddenly realized at a symposium on EXAFS that 'making the lattice spacing larger by adding B might not improve magnetism.'"

(3) Development of an inorganic microcapsule (Nakahara at Government Industrial Development Laboratory, Osaka)—Mr Nakahara developed a preparation method of new spherical inorganic grains by applying the boundary surface reaction method (a method of preparing polymer microcapsules).

During surface chemistry research on the surface of inorganic particles, Mr. Nakahara believed the need for uniform particles and embarked on the manufacture of micro-balloons. The application of the manufacturing principle of polymer microcapsules to inorganic aqueous solution reaction led to the discovery of the manufacturing technique of a new class of "inorganic micro-balloon." Used as a slow-releasing, functional material, the microcapsule was commercialized. The successful development is due to steady research on surface chemistry, good leaders and managers, and support from universities and enterprises.

(4) Development of WA 310 and 320 binders (joint work with private sector).

[continued]

- (5) A casting method in which silicon rubber is used in place of a core vulnerable to collapse (getting a hint from monodirectional casting).
- (6) Study on the relationship between the grain boundary in zinc oxide varistor and grain gave a hint to the development of a low thermal expansion coefficient and high-strength material.
- (7) Development of a transparent alumina (lucalox).
- (8) Development of SiAlON.
- (9) Oxide superconductor.
- (10) X-ray diffraction.
- (11) Abnormal deformation of zirconia was discovered in the course of conducting research on creep in heat-resistant structural ceramics. Although perplexing, it struck me that the problem may be related to the superplasticity phenomenon observed in metallic materials, and the flash of imagination opened the way for a rich variety of applications. The phenomenon got the attention of researchers in fields other than ceramics, and support was obtained from them.

Private sector

(40/60)

- (1) Development of an efficient volume production method of imides—Learning by chance that ceramic researchers use surface reaction in polymer synthesis, the technique was applied in the synthesis of inorganic materials.
- (2) Discovery of transistors.
- (3) Development of high-strength ceramics (JOURNAL OF THE JAPAN FINE CERAMICS ASSOCIATION, 1990, No 5)—When fabricating composites of silicon carbide and silicon nitride, in an attempt to alter the ratio of grain diameters between additives and matrix, specimens were prepared by altering the sintering conditions and grain diameters of the raw materials.
- (4)
 - Esaki tunnel diode
 - Shockley transistor
 - High-temperature superconductors by Mueller and Bednorz

[continued]

(5) Professor Hideo Honma (Kanto Gakuin University)—Professor Honma has many achievements to his credit in the plating field, and his ideas are creative.

(6) Light control film—When dealing with light hardening resins for use as an intermediate layer for glass, I discovered by chance a slightly shaded film when seen from an oblique direction. It was unfit as the targeted film, but I persistently sought the cause of the film.

(7) Discovery of a technique that enables organic particles to be mixed inside SiO_2 —An attempt to mix an organic pigment in an aqueous solution for liquid-phase film growth (SiO_2) was successful.

(8) ZNR (different grain phases/ Bi_2O_3 solid phase grains (ZnO))—A mistake in sintering in an electric oven by the field people led to the discovery of abnormal properties.

(9) Cases at TDK

- Spurred at Esaki diode, experiments were conducted to see how much impurities were permissible for high-purity BaTiO_3 semi-conductors prepared by the oxalic acid method. The results showed the effects of adding trace amounts of Mn, Fe or Cr, opening the way for the practical use of PTC.

- To counter DuPont's exclusive patent for high-performance magnetic powder (CrO_2), attempts were made to develop indigenous magnetic powder. A breakthrough was obtained by improving the surface properties of magnetism of iron oxide and by adding additives, thereby succeeding in its development.

(10) Kevlar fiber—A mistake in the preparation of solvent helped the resin to be dissolved, thus opening the way for the resin's fabrication into fibers.

(11) An example at Adamatech Co.—A pearl-like SiO_2 (submicron) synthesized while trying to develop a synthesis method of particles of Si_3N_4 .

Aim: $\text{Si} + 4\text{NH}_3 \rightarrow \text{Si}_3\text{N}_4 + 6\text{H}_2$

Result: $\text{Si} + \text{O}_2$

In addition, synthesis of Al_2O_3 and Fe_2O_3 is possible.

(12) I was very impressed by the fighting spirit of the inventors in the December 1990 issue of INVENTION. Why don't you take inspiration from the episodes?

[continued]

(13) While conducting research on piezoelectric materials, I usually fabricate a device by pasting two piezoelectric plates with electric potential sandwiched in between. I discovered a device in which only one piezoelectric plate warps.

(14) When synthesizing high-purity ZrSiO_4 , adding trace amounts of natural zircon enables us to obtain high-purity zircon.

(15) Preparation of machinable ceramics by the sol-gel method. Although the sol-gel method may be nothing new by itself, the combination of several element technologies can lead to a unique technology.

(16) It was discovered by Prietley that viscous minerals are effective as a catalyst in synthesizing ethylene from ethyl alcohol. This could have been predicted more readily if it had been known that clay minerals have a large specific surface area, that aluminum silicate has properties similar to solid acid, and that pores are the structures generated inside crystals.

(17) Grain orientation and low expansion by extrusion forming of cordierite honeycombs.

(18) Y_2O_3 has been found to be effective as an additive to AlN sintering. While I was working for Toshiba Corp., we had someone studying oxides of rare-earth elements, and I found Y_2O_3 to be highly effective (according to assistant Professor Yoneya at Yokohama National University).

(19) Around 1970, we started research and development of cement using gypsum. We accomplished the processing method of then rarely-used "auin" clinker, which opened the way for the development of feedstock materials for many specialized cements, such as GRC cement and solidifying cements.

Q7-(2): Proposals of requests for environments of research systems that will foster unique ideals and flashes of imagination

Universities and colleges:

1. Luxury of abundant resources (time, money, organization, climate)
 - A forum for free discussion.
 - A research forum where one is free from the pressure to write a paper.
 - A research reorganization where one feels freedom of action.
 - Social support that allows one to pursue research energetically but at one's own pace (financial and spiritual support).
 - Too busy because of reductions in manpower.
 - Opportunities in which persons with backgrounds can talk of "dreams" and execute them. A systematic and financial support system that enables one to implement his dream.
 - Understanding the actual state of advanced industry.
 - Freedom of research and "not being too busy." Opinions of subordinates must be given an equal opportunity for discussion.
 - Giving those people gifted with ideas and flashes of imagination a forum for free research.
 - The closed and conservation personnel management system must be abolished.
 - Unique and creative ideas are born of abundance.
 - Basic studies must be undertaken on a long-term basis.
 - The Ministry of Education policy of not allowing individual universities' self-reform initiatives is a problem.
 - Luxury in which one can indulge in various ways of thinking.
 - A carefree and relaxed environment where an idea can bear fruit.
 - Research planning with much latitude.
 - An idea must grow through brainstorming.
2. Exchanges with other fields
 - Joint research must be undertaken and promoted in a broad range of fields.
 - An increase in exchanges among different fields of science.
 - An inflow of needs from society (enterprises) to universities, and an outflow of seeds and basic studies to society.
 - Collaboration between industry and academia.
 - Interdisciplinary exchanges.
 - The ceramics field is an interdisciplinary field.
 - A forum where researchers from different fields can have an exchange and can cooperate.
 - An exchange among government, academia, and industry.
 - An opportunity to have exchanges and discussions with researchers from different fields. "Pure culture" should be avoided.
 - An effective encounter between needs and seeds.
 - To expand interest into other fields (medicine, biology, etc.).

[continued]

3. Research funds, equipment, time, and structure

- Supporting basic research on a long-term basis.
- Beefing up various measuring equipment.
- Ample research funds.
- Long-term research on a few select research themes.
- Large-scale projects.
- Bottom-up rather than top-down.
- The shortages of funding for education bode ill for the future.
The shortages of funding at local universities are getting worse.
- Support structure (technicians, workrooms, machinery, analyses).
- An environment where experiments can be readily undertaken.
- There must be an environment where experiments can be conducted readily and speedily.
- A foundation where the elements of heterogeneity, fluidity, and atypicality are accepted. Replacement of the old with the new in research institutes.
- Securing enough funds for research.
- How about establishing an association of young ceramics researchers?
- Inviting young foreign researchers.
- An improvement on the system under which researchers are sent overseas for research.

4. Education and training

- Improvements in the curriculum.
- Freeing the curriculum in universities.
- A thorough training in basic studies.
- Research on educational techniques.
- A review of the way in which graduate school education is being given (basic studies up to the master's course).
- Rationalization of high school education.
- Sending more students who can score fairly good marks without being a booster of the university.
- An educational environment in which one's personality can flourish and his sense of good taste is cultivated.
- The "common sense" of professors and experienced people is hindering the buds of the young from flourishing.
- One's seniors must be broadminded and tolerant.
- The government and enterprises must make efforts to train talented people.
- It is necessary that young people be given an opportunity where they can display their abilities to the highest degree.
- Efforts should be made to train talented people.
- Specific education for brilliant children.

[continued]

5. Evaluation

- Brief and simple progress reports on research (long explanations are often sought).
- Research must be judged over a span of two years.
- The method of evaluating budding research must be revised.
- Due appreciation should be given to the researcher as a human when evaluating him.
- Research is often conducted as a copy of what foreign researchers are doing, but an environment must be fostered where doing the type of research which no one else is doing will be highly evaluated.
- It is wrong to expect short-term gains in research.
- Basic research is given too low an evaluation.

6. Treatment improvements

- Increased research funds for students, assistants and assistant professors who conduct much of the research. Also, scholarships are wanted.
- Researchers are poorly treated.
- Liberation from chores.
- About a month of leave, away from research or chores.
- A substantial strengthening of the grant-in-aid for the research system.
- Increased transfer of authorities.
- Salaries must be increased so that the teaching ranks can recruit outstanding students.

7. Self-enlightenment

- Efforts.
- To maintain the desire to be creative at all times.
- The most important thing is for a researcher to be burning with the desire to pursue research.
- Qualities demanded of a researcher as a human being—a curiosity in a broad range of affairs, the ability to see the true nature of things, free spirit, and another embodiment of one's self (to be able to see one's self objectively).
- To be always mindful of what the problems are and how to solve them.
- A researcher should resolutely proceed toward his goal step by step, rather than casting around for a quick result, distracted by successes of people around him.

8. Others

- Research on a support system that helps one to come up with ideas.
- Removal of the wall between the Ministry of International Trade and Industry and the Ministry of Education research frameworks.
- Databases

National and public laboratories

1. Luxury of abundant resources (time, money, organization, climate)
 - Enough research time, facilities, and research related pressure.
 - Enough time so that one can study literature.
 - Because of the pressure to come up with a tangible result, I am too hard pressed to study things deeply.
 - A unique idea or a flash of imagination comes not from well-planned research but from research that has run off course.
 - Atmosphere of freedom.
 - An environment that is tailored to the personality of the researcher.
 - If there is no "place where discussions can be held freely," even an excellent staff will lose half of its prowess.

The attainment of the goal is next to impossible in the real world. (Even a simple odd-man-out will spoil the atmosphere.)

 - A good idea will never come out of a controlled research structure. Beautiful flowers are occasionally found in the sideways.
 - Continuity in research.

2. Evaluation

- A research project that failed to produce results each passing year but is continued for several years is given a low evaluation.
- An evaluation from a long-term rather than short-term perspective.
- The administrator is too persistent in demanding a short-term result.
- An evaluation should be given not from the yardstick of how many papers a researcher has published but should be given based on their contents. (Administrators rank low in their ability to evaluate.)
- Evaluations are not so demanding when compared with those in industry.
- A proper and just evaluation will always lead to a good result.
- Social factors that affect evaluation of the results (supervisors who decide to start commercialization, top officials of companies).

3. Research funds, equipment, personnel, and structure

- Creative research can only come out of a structure where much importance is attached to basic research.
- The existence of a support system (human resources).
- An increase in pseudo managerial duties.
- "Make money available but stay away from interfering."
- The research environment for researchers is too poor (such as non-availability of ones own laboratory, etc.).
- A review should be done for possible reform of the system in which to get funding for a research project; planning would have to be drafted two years in advance.
- Abolish the indiscriminate egalitarianism for budget allocation.
- To bring overall harmony with diversification of research organizations.
- Managers who will ensure the continuity of research, and research budget.

[continued]

4. Education and training

- Education of the young who will shoulder research in the next generation.
- Education based on a demerit system will not be able to train executive people.
- Unless you have an eye to see things through, you will fail to direct talent.

5. Exchange with different fields

- An encounter between needs and seeds. We have a bulletin board for industry-related information.
- Human exchanges (information on needs and seeds are forthcoming).
- Link between people who produce materials and people who use those materials.

6. Others

- Paper work is not rationalized.
- Getting rid of preconceptions.
- I have a doubt about the increasing trend toward survey research.

Private sector

1. Exchanges with other fields

- Attending meetings and lectures given by academic societies in other fields of science.
- Organizing mixed teams with people from other fields of science.
- Promotion of multitasks.
- Exchanges of opinions with people from fields of science, with one's seniors and juniors; holding study sessions.
- Interchanges with government research organizations, including dispatching people to other offices.
- Joint research among academia, government, and industry.
- Exchanges with people from other industries.
- Approaches transcending the barriers of academic groupings and industries.
- Research groups of people with different mentalities and characters.
- To obtain knowledge of fields other than one's specialty.
- To create an environment where young researchers can readily seek the opinions and ideas of professionals in various fields.
- A forum for technical exchanges is needed. The current academic societies' and associations' activities must be reexamined for possible reform.
- To bring together researchers from different specialized fields.
- To cross-reference needs with seeds.

[continued]

2. Luxury of abundant researchers (time, money, organization, and climate)

- An environment where time and financial support are available for initial-stage experiments.
- A nonbureaucratic climate that accepts free ideas and actions.
- A good balance between luxury and stress (delivery and presentation).
- High degrees of freedom in the selection of research themes.
- In corporate research labs the pace of research is not so leisurely as that in government labs.
- Promotion under the desk.
- An environment is needed where a researcher can do anything he likes to obtain data on ceramics. With ceramics, all we can do is just try.
- It is necessary to sit down with university professors and start from theoretical studies. (One idea is to organize a research group that has a wide latitude in decisionmaking under a joint research laboratory program.)
- Ample time and ample funding for research.
- To give a researcher a small degree of luxury whereby in working toward his organization's goal, he can indulge in his own interest.
- Not to seek short-term results.
- The Japanese have a tendency to censure others' originality.
- An environment where the researcher is free from not only constraints but also from the pressure of time, coupled with a research system staffed by a supervisor who accepts the aforementioned atmosphere.
- Young researchers should be given some long periods of time so that they can pursue their research freely.
- I would like to have an environment where a researcher is permitted to pursue a research theme of his choice, if he happens to have one. I need about a day of escape per month when I can be completely free from the pressure of research.
- An environment is needed where the researcher can pursue his research with a strong will and with no fear of failure and yet at his own pace.

3. Self-enlightenment

- Not to be burdened with any preconceived opinion.
- Acquisition of basic knowledge and information.
- Training in the use of the right sphere of the brain.
- Steady research according to the basics, with no reliance on simple luck.
- Training in enhanced concentration.
- A spirit of trying something different in liberating one's self from conventional wisdom.
- "Obsessive zeal" on the part of the researcher.
- A strong will to pursue creativity.
- The top management's trust in researchers.
- It all boils down to what professor Yanagita says, "serendipity" (work hard, and study hard—the importance of basic science).

[continued]

- Learn both basics and applications.
- Raising the qualities of both individuals and organizations.
- Giving a more detailed theoretical explanation to the origin of matter.
- Ultimately, it all depends on the individual researchers' abilities.
- Keep the scope of your mental antenna wide open, and maintain your curiosity.
- Try to absorb knowledge of things in fields other than your specialty.

4. Research money, equipment, staff, and structure

- Improvements in the experimental equipment and analysis instruments.
- As for the organizational structure of research, the requirement is that it is being led by a person of high vision and high motivation. I have always been told, "do what others cannot do, and become the first person in the world to do it."
- The abilities of a person or persons who design the environment and research system are important.

5. Others

- A database for "flashes of imagination," complete with computer backup.
- It is difficult. We will do only what we can do.
- The seniority system should be abolished.
- An important thing is to create an atmosphere and an evaluation system in which cases of failures are evaluated and whatever merits can be gleaned of those examples are put to good use.
- Since R&D is highly dependent on the individual, how about surveying individual researchers' blood types? Type B's find treasure troves through flashes of imagination, while type A's employ the carpet bombing method.
- Don't gather too much data.
- University and government laboratories should undertake research of higher originality.
- Although I, as a member of management, am thinking it over day and night, there is no quick solution.
- You should never settle for defects and problems which exist in currently available products as essential qualities, but keep dreaming of something better.
- By understanding where society is heading, you should try to grasp what demands await to be met.
- If a discovery is made, try to emphasize what a meaningful discovery it is.

- END -

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